*J. Math. Pures Appl.* 80, 7 (2001) 701–738

S0021-7824(01)01213-2/FLA

# CONSTRUCTION, STRUCTURE AND ASYMPTOTIC APPROXIMATIONS OF A MICRODIFFERENTIAL TRANSPARENT BOUNDARY CONDITION FOR THE LINEAR SCHRÖDINGER EQUATION

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Manuscript received 24 January 2001

ABSTRACT. – A transparent boundary condition for the two-dimensional linear Schrödinger equation is constructed through a microlocal approximation of the operator associating the Dirichlet data to the Neumann one in a "$M$-quasi hyperbolic" region. Several quasi-analytic characterization results concerning the asymptotic expansion of the total symbol of this operator in a subclass of inhomogeneous symbols with a quasi-polynomial-like structure are stated. In particular, a high-frequency control giving the behavior of these symbols is precised. It highlights the way of how to derive some consistent asymptotic artificial boundary conditions involving fractional derivatives with respect to the time variable by approximating the micro-transparent condition in the high-frequency regime. These approximate conditions are local according to the space variable and should lead to some efficient and accurate numerical simulations if they are used to truncate the unbounded domain of propagation. © 2001 Éditions scientifiques et médicales Elsevier SAS

*Keywords:* Schrödinger equation, Transparent boundary condition, Artificial boundary condition, Micro-operator, Dirichlet–Neumann operator

## 1. Introduction

We consider the Schrödinger linear equation free from any potential and classically sets in the unbounded domain $\mathbb{R}_x^2 \times \mathbb{R}_t$:

$$\text{(1)} \qquad \begin{aligned} &L(\partial_x, \partial_t)u = (\mathrm{i}\partial_t + \Delta)u(x,t) = 0, \quad (x,t) \in \mathbb{R}_x^2 \times \mathbb{R}_t, \\ &u(x,0) = u_0(x), \quad x \in \mathbb{R}_x^2, \end{aligned}$$

with $u_0 \in H^1(\mathbb{R}_x^2)$ with a compact support $\widetilde{\Omega}$. From a physical viewpoint, problem (1) naturally arises in quantum mechanics, and with some additional nonlinear terms, in nonlinear waves propagation as for instance in the propagation of a laser beam in a media with a refraction index

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sensitive to the wave amplitude, in the propagation of an aquatic wave at the free surface of an ideal fluid or also in plasma waves.

The numerical approximation of (1) is usually made in a truncated domain $Q = \Omega \times [0, T]$, with $\widetilde{\Omega} \subset \Omega \subset \mathbb{R}^2$ of boundary $\Gamma = \partial\Omega$ regular enough and $T > 0$. To have a solution $v$ in $Q$ which exactly coincides with the restriction to $Q$ of the solution $u$ of the Cauchy problem (1), a suitable boundary condition has to be imposed on $\Sigma = \Gamma \times [0, T]$. This so-called *exact* condition is defined through a non-local (both in space and time) pseudodifferential operator $\mathcal{B}^+ = \mathcal{B}^+(x, \partial_x, \partial_t)$ giving rise to the boundary condition:

$$\mathcal{B}^+(x, \partial_x, \partial_t)v(x, t) = 0, \quad \text{on } \Sigma.$$

In fact, it can be proved that such a condition can be expressed by favouring the normal derivative trace operator $\partial_{\mathbf{n}}$ and the Dirichlet–Neumann (DN) operator $\Lambda$ giving the Neumann data of $v$ from the Dirichlet one, i.e. $-\partial_{\mathbf{n}} v_{|\Sigma} = \Lambda v_{|\Sigma}$, $\mathbf{n}$ designating the outwardly directed unit normal vector to $\Omega$. Operator $\Lambda$ is a first-order non-local pseudodifferential operator. Next, we propose to construct an approximate solution $v$ of $u$, satisfying $u - v \in \mathcal{C}^\infty([0; T] \times \overline{\Omega})$, on a finite region $\Omega$ with a regular curved boundary $\Gamma = \partial\Omega$ and solution to:

$$\begin{aligned}
&L(\partial_x, \partial_t)v = 0, \quad (t, x) \in [0; T] \times \Omega = Q, \\
&v_{|t=0} = u_0, \quad x \in \Omega, \\
&(\partial_{\mathbf{n}} + \Lambda)v = 0, \quad (t, x) \in [0; T] \times \Gamma = \Sigma.
\end{aligned}$$

Among the approaches developed for the construction of an exact condition, one of the most efficient is due to Grote and Keller [15] in the context of the scattering of an acoustic wave. It is well-known that their conditions [14,16–21] give some accurate results since, from their construction itself, they only generate some small reflections. In return to this good precision, this approach, restricted to a circular boundary, leads to some quite expensive computational costs due to the presence and evaluation of a convolution kernel. Nevertheless, the use of recent evaluation algorithms of these kernels [1] may improve the speed of these methods. Furthermore, at the best of our knowledge, the special case of the Schrödinger equation has not still been explicitly considered even if Hagstrom gives the outlines in [19].

An alternative to this approach consists in replacing the exact condition characterized by the operator $\Lambda$ by an approximate condition which does not generate any reflection at the fictitious boundary. Consequently, this condition is usually called *transparent* and is such that

$$T^+(x, \partial_x, \partial_t)\tilde{v}(x, t) = 0, \quad \text{on } \Sigma,$$

where $\tilde{v}$ is an approximation of $v$ in a band of frequencies. The associated operator $T^+$ is said to be a *transparent* operator. Several methods has been devised to directly treat this condition which similarly to the exact condition is also of non-local type. On this subject, let us mention the construction of discrete transparent boundary conditions by Schmidt and Yevick [32] and next improved by Arnold and Ehrhardt [4] or also the approach developed by Baskakov and Popov [5] and based on the use of finite difference schemes to approximate the fractional transparent operator, these two approaches being derived for a plane boundary. However, even if these two methods give rise to some accurate results, their application can be limited because of their non-local character. As a natural consequence is posed the question of how to construct a local (or nearly local) boundary condition approximating in a certain sense the transparent condition.

The most widely used approach to realize it has been originally introduced by Engquist and Majda [11,12] who make use of the theory of reflection of singularities [30] to construct a non-local transparent boundary condition for the wave equation which reproduces the singularities of the solution. The keystone of the conception of the associated transparent operator is contained in a factorization theorem due to Nirenberg [31]. Next, approximate local boundary conditions are deduced from this condition by the use of Padé approximants (or more generally from some paraxial approximations [10,24]) of the symbol of the transparent operator. One of the other interesting points of this approach is that similar results can be obtained for general pseudodifferential systems by using a microlocal diagonalization theorem [2,11,12,34,35]. This is the approach that we consider in this paper.

To our knowledge, the first attempt of application of this approach to the Schrödinger equation is due to Shibata [33] who derives some local conditions in the one-dimensional case. Next, this work has been extended to the two-dimensional half-space by Kuska [27]. More recently, in [9], Di Menza has written following this process and using a physical interpretation some paraxial artificial boundary conditions for a plane boundary $\Gamma$. In [13], Fevens and Jiang also give some approximate conditions both for the two and three-dimensional case well-adapted to some finite-difference schemes. Nevertheless, all these studies are made in a simplified framework for the mathematical analysis of the transparent condition: the half-space case. This particular geometrical configuration allows to make an analysis of the transparent condition by the Laplace–Fourier transform which in fact hides the true nature of the arguments to derive it. Moreover, these conditions are restricted to a plane boundary and can generate some spurious reflections due to some corner-like singularities if they are directly set on a more general curved boundary. Some additional corner conditions quite difficult to obtain must be imposed. Furthermore, to consider a more regular boundary $\Gamma$, as for, e.g., a circular one, appears to be more in accordance with the nature itself of the prospected solution to (1). We propose in this paper a detailed mathematical analysis of the construction of the transparent operator on a curved boundary for the two-dimensional space Schrödinger equation. It will be shown that the symbol of this operator possesses some interesting algebraic properties well-suited for their paraxial approximations (problem that will be treated in a subsequent work).

This paper is organized as follows. In Section 2, we begin by recalling some useful results about the $M$-quasi homogeneous symbolic calculus of Lascar [29] and notably used by Boutet de Monvel [8] to study the propagation of singularities for Schrödinger-like equations. This particular calculus allows to give an account in a precise way of the repercussion on the pseudodifferential calculus of the inhomogeneity present between the space and time covariables for the Schrödinger equation (apparent for instance in the dispersion relation). Next, we show how to write a transparent operator $T^+$ for a curved boundary working in a system of generalized coordinates associated with $\Gamma$. We explain the sense to give to this operator relying on Lascar's [29] results in order to precise the mathematical background. In fact, the operator is constructed in its region of hyperbolicity, called here $M$-quasi hyperbolic, where it is a "quasi-homogeneous" pseudodifferential operator (in the sense of [29]). Moreover, it can be microlocally rewritten by favouring the normal derivative operator, i.e.

$$T^+ = \partial_{\mathbf{n}} + \mathrm{i}\widetilde{\Lambda^+},$$

where the operator $\widetilde{\Lambda^+} = \widetilde{\Lambda^+}(x, \partial_t, \partial_x)$ is a first-order microdifferential operator constructed as an approximation of the DN operator $\Lambda$. This is a consequence of a factorization theorem for the Schrödinger operator analogous to the result of Nirenberg[31] for classical pseudodifferential operators. Moreover, we establish some differential relations allowing to recursively compute the asymptotic expansion of the total symbol of $\widetilde{\Lambda^+}$. In a third section, a subclass of $M$-quasi homogeneous symbols with a simple "quasi-polynomial" algebraic structure is introduced. Then, we prove that operator $\widetilde{\Lambda^+}$ has an asymptotic expansion in this class. Moreover, this characterization gives an asymptotic control of the symbolic expansion in the high-frequency zone. This brings to the fore the existence of a symbolic polynomial $P$. So, we state in Section 4 several results concerning some "quasi-analytic" characterizations of $P$. They give explicitly the form of this polynomial if certain rational coefficients are computed. This can be done by the recursive relation previously derived. In particular, it turns out that the operator $\widetilde{\Lambda^+}$, even if it is not differential, owns a simple form for its approximation. We give a proof of these results which is based on a very precise handling of the whole symbolic calculations required for the evaluation of symbols defining the asymptotic expansion of the transparent operator. We finally present in Section 5 a complete analysis for the construction of some consistent asymptotic artificial boundary conditions of arbitrary order on any fictive convex boundary $\Gamma$. These conditions are *non-local in time* but have the very interesting property of being *local according to the space variable*. Finally, we explicitly give the first, second- and third-order consistent conditions which appear as being useful for some future numerical computations. Other possible approximations may lead to other families of suitable artificial boundary conditions.

## 2. Microlocal construction of the transparent operator

### 2.1. Notations and $M$-quasi homogeneous symbolic calculus

This subsection is devoted to some useful recalls particularized for our specific problem on the essential notations and results concerning the pseudodifferential analysis for symbols of a fixed order and non-isotropic growing at infinity. We refer to [29] for more complete and general results.

Let $M = (1,2)$. We consider an open set $X$ of $\mathbb{R}^2$ and we introduce for the particular pair $M$ the dilatations $\mathbb{H}_M^\mu$ defined by:

$$\forall \mu > 0, \quad \mathbb{H}_M^\mu(x,\xi) = \big(x, \mu\xi_1, \mu^2\xi_2\big),$$

where $x = (x_1, x_2)$ is a point of $X$ and $\xi = (\xi_1, \xi_2) \in \mathbb{R}^2$ stands for the covariable of $x$. In the sequel, an open set $\mathcal{C}$ is called an anisotropic $M$-cone if it is stable by the action of $\mathbb{H}_M^\mu$ for every $\mu > 0$. This notion extends the one of a conic open set usually used to microlocalize a classical pseudodifferential operator. Now, let $f$ be a regular function. Then, $f$ is said to be $M$-quasi homogeneous of degree $m$ if $f \circ \mathbb{H}_M^\mu = \mu^m f$, $\mu > 0$. From now on, a $M$-quasi homogeneous pseudodifferential operator of order $m$, denoted by $A \in OPS_M^m$, is defined as an operator with a total symbol $a(x,\xi)$ admitting an asymptotic expansion in $M$-quasi homogeneous symbols:

$$a(x,\xi) \sim \sum_{j=-m}^{+\infty} a_{-j}(x,\xi),$$

where functions $a_{-j}$ are some $M$-quasi homogeneous symbols of degree $-j$. This will be denoted by $a \in S_M^m$. A symbolic calculus can next be associated with this class of operators [29].

*Remark* 1. – In [23], Halpern and Rauch consider the inhomogeneous calculus stated in [6,7] to characterize the pseudodifferential transparent operator for the convection–diffusion equation.

### 2.2. The transparent operator

We are interested here in the local contruction of the transparent operator $T^+$. We show that it can be microlocally rewritten by favouring the normal derivative operator, i.e.:

$$T^+ = \partial_{\mathbf{n}} + \mathrm{i}\widetilde{\Lambda^+},$$

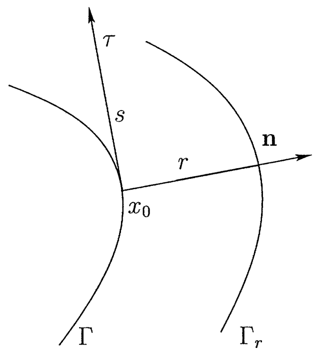


Fig. 1. System of generalized coordinates.

where $\widetilde{\Lambda^+} = \widetilde{\Lambda^+}(x, \partial_t, \partial_x)$ is a first-order microdifferential operator. Its construction is based on a microlocalization of the DN operator. As a consequence, a new writting of the transparent condition is proposed as:

$$\big(\partial_{\mathbf{n}} + \mathrm{i}\widetilde{\Lambda^+}\big)v = 0, \quad \text{on } \Sigma.$$

In fact, the local expression of the normal derivative operator $\partial_{\mathbf{n}}$ on the boundary $\Sigma$ results from a study of the backward and forward bicharacteristics associated with the Schrödinger equation.

Let $x_0 \in \Gamma$ and $(\mathbf{n}(x_0), \boldsymbol{\tau}(x_0))$ be the anticlockwise directed system of generalized coordinates, where $\boldsymbol{\tau}$ is the unitary tangent vector at point $x_0$ (Fig. 1). In this system, the local coordinates of a point near $x_0$ are denoted by $(r, s)$. Variable $r$ designates the normal variable along the unit normal vector $\mathbf{n}$, where $r \in \,]-\varepsilon, \varepsilon[$, $\varepsilon$ being sufficiently small, whereas $s$ is the curvilinear abscissa along $\Gamma$. Consequently, $\partial_{\mathbf{n}(x_0)}$ can be defined as the limit of $\partial_r$ when $r$ tends to 0. The stationnary part $\Delta$ of the Schrödinger operator can then be rewritten as: $\Delta = \partial_r^2 + \kappa_r \partial_r + h^{-1}\partial_s(h^{-1}\partial_s)$, where $\kappa_r = h^{-1}\kappa$ is defined as the curvature on the parallel surface $\Gamma_r$ to $\Gamma$ and $h$ is the parameter $h(r,s) = 1 + r\kappa$. The operator $L = L(r, s, \partial_r, \partial_s, \partial_t)$ is so a second-order operator with respect to $\partial_r$. The main difficulty is now to factorize $L$ to extract the operator $\partial_r$. As in [31], we make use of the symbolic calculus.

Let us define $\tau$, $\rho$ and $\xi$ as the covariables associated respectively with $t$, $r$ and $s$. In the sequel, the factorization theorem only holds in a relevant subset of frequencies. To precise it, let us introduce the following notations. Let $T^*(\Sigma)$ be the cotangent bundle at the boundary. It can be divided into three parts. Let us denote by $\pi$ the canonical projection of $T^*(\mathbb{R}^3)$ onto $\mathbb{R}^3$ and $\Pi$ the canonical projection defined by $\Pi : \pi^{-1}(\Sigma) \cap T^*(\mathbb{R}^3) \to T^*(\Sigma)$ which associates with a point $(0, s_0, t_0, (\rho_0, \xi_0), \tau_0) \in T^*(\mathbb{R}^3)$ the point $\zeta_0 = (s_0, t_0, \xi_0, \tau_0) \in T^*(\Sigma)$. Let us introduce $p_2$ as the characteristic polynomial of the Schrödinger equation: $p_2(0, s_0, t_0, \rho_0, \xi_0, \tau_0) = -\rho_0^2 - (\xi_0^2 + \tau_0) = 0$. This second-order equation with respect to $\rho_0$ admits two roots $\rho_0^{\pm} = \mp(-(\xi_0^2 + \tau_0))^{1/2}$. In order to precise the inhomogeneity appearing in $\rho_0^{\pm}$, we use the quasi-homogeneous symbolic calculus established in [29]. Each symbol $\rho_0^{\pm}$ is $M$-quasi homogeneous of degree 1. To characterize the set of frequencies for which the factorization holds, we have to define the following classification:

DEFINITION 1. – *Let* $\mathrm{car}_M(L) = p_2^{-1}(0)$ *be the characteristic M-cone* [29]. *The M-quasi hyperbolic zone* $\mathcal{H}$ *is the set of points* $\zeta_0 = (s_0, t_0, \xi_0, \tau_0) \in T^*(\Sigma)\backslash\{0\}$ *such that*:

$$\#\Pi^{-1}(\zeta_0) \cap \mathrm{car}_M(L) = 2,$$

*that is* $\mathcal{H} = \{(s_0, t_0, \xi_0, \tau_0) \in T^*(\Sigma)\backslash \tau_0 + \xi_0^2 < 0\}$. *Likewise, the* $M$*-quasi elliptic zone is defined as*:

$$\#\Pi^{-1}(\zeta_0) \cap \mathrm{car}_M(L) = 0,$$

*or also* $\mathcal{E} = \{(s_0, t_0, \xi_0, \tau_0) \in T^*(\Sigma)\backslash \tau_0 + \xi_0^2 > 0\}$. *Finally, the third complementary zone called* $M$*-quasi glancing is* $\mathcal{G} = T^*(\Sigma)\backslash(\mathcal{E} \cup \mathcal{H})$.

As in the case of a linear hyperbolic operator [26,28,30,34], the set $\mathcal{E}$ does not contribute to the propagative part of the solution and physically represents the region of evanescent rays, i.e. with a real phase and exponentially decreasing (cf. [9] for the proof in the half-space case). Under the assumption that the open set $\Omega$ is strictly convex and of positive curvature, the zone $\mathcal{G}$ corresponding to the propagative tangential part of the solution is reduced to $\{0\}$. Finally, we only have to characterize the reflection phenomenon in the anisotropic $M$-cone $\mathcal{H}$.

Let $\gamma^{\pm}(\theta) = (r(\theta), s(\theta), t(\theta), \rho(\theta), \xi(\theta), \tau(\theta))$ be the two $M$-bicharacteristic strips associated with the initial conditions $\gamma^{\pm}(0) = (0, s_0, t_0, \rho_0^{\pm}, \xi_0, \tau_0)$, that is the integral curves solutions of the Hamilton equations [29]. They carry the singularities of the approximate solution $v$. Then, for $r$ sufficiently small and setting in a $M$-conic neighborhood of $\mathcal{H}$, operator $L$ admits two distinct real roots $\rho^{\pm}(r, s, t, \xi, \tau) = \mp(-(h^{-2}\xi^2 + \tau))^{1/2}$. Next, the forward $M$-bicharacteristic strip $\gamma^+$ is selected by the condition $\dot{r} > 0$. From the Hamilton equations, it is equivalent to have

$$\dot{r} = \frac{\mathrm{d}r}{\mathrm{d}\theta} = \partial_\rho p_2 = -2\rho > 0.$$

Thus the choice of $\rho^+$ characterizes $\gamma^+$ which carries the outgoing ray.

*Remark* 2. – The assumption about the strict convexity of the computational domain $\Omega$ leads us to suppose that the curvature satisfies locally $\kappa > 0$. Consequently, a straightforward calculation gives:

$$\rho^+ < \rho_0^+ \quad \text{and} \quad \rho_0^- < \rho^-$$

and so ensures that the two rays have been well splitted.

Essentially, the principal symbol of $L$ has been microlocally factorized in $\mathcal{H}$. By recursivity, we get a complete factorization of the total symbol of $L$ in the $M$-quasi hyperbolic zone.

THEOREM 1. – *There exist two pseudodifferential operators* $\Lambda^{\pm} = \Lambda^{\pm}(r, s, t, \partial_s, \partial_t) \in OPS_M^1$, *smooth with respect to* $r$, *such that the following factorization holds*:

$$L(r, s, \partial_r, \partial_s, \partial_t) = \big(\partial_r + \mathrm{i}\Lambda^-(r, s, \partial_s, \partial_t)\big)\big(\partial_r + \mathrm{i}\Lambda^+(r, s, \partial_s, \partial_t)\big) + R(r, s, \partial_s, \partial_t), \tag{2}$$

*where the symbol* $\sigma(R) \in S_M^{-\infty}$ *and the principal symbol* $\lambda_1^{\pm} \in S_M^1$ *of* $\Lambda^{\pm}$ *is equal to* $\rho^{\pm}$ *in a* $M$*-conic neighborhood of* $\zeta_0 \in \mathcal{H}$, *for any* $\rho$.

*Proof.* – The proof is constructive and essentially relies on the implicit determination of the operators $\Lambda^+$ and $\Lambda^-$ from their respective symbols $\lambda^+$ and $\lambda^-$ in $S_M^1$.

Consider the following factorization of the Schrödinger operator in a $M$-conic neighborhood of the $M$-quasi hyperbolic region:

$$L(r, s, \partial_r, \partial_s, \partial_t) = \big(\partial_r + \mathrm{i}\Lambda^-(r, s, \partial_t, \partial_s)\big)\big(\partial_r + \mathrm{i}\Lambda^+(r, s, \partial_t, \partial_s)\big) + R. \tag{3}$$

Introduce $\{\lambda_{-j}^{\pm}\}_{j=-1}^{+\infty}$ as being the asymptotic expansions in $M$-quasi homogeneous symbols $\lambda_{-j}^{\pm}(r, s, \tau, \xi)$ of the total symbols $\lambda^{\pm}$ in the anisotropic class $S_M^{-j}$. Expanding expression (3) and using a few manipulations on the operators [3], we get the relation:

$$L = \partial_r^2 + \mathrm{i}\big(\Lambda^+ + \Lambda^-\big)\partial_r - \Lambda^-\Lambda^+ + \mathrm{i}\mathrm{Op}\big(\partial_r\lambda^+\big) + R, \tag{4}$$

where $\mathrm{Op}(a)$ designates the operator whose symbol is $a$. By identification of the terms appearing in front of the radial derivative operator in the Schrödinger equation in local coordinates:

$$L(r, s, \partial_r, \partial_s, \partial_t) = \partial_r^2 + \kappa_r\partial_r + h^{-1}\partial_s\big(h^{-1}\partial_s\big) + \mathrm{i}\partial_t$$

with the ones in (4) and next using their symbolic expressions, we can conclude that both $\lambda^-$ and $\lambda^+$ are solutions of the symbolic system:

$$\begin{aligned} &\mathrm{i}\big(\lambda^+ + \lambda^-\big) = \kappa_r, \\ &\mathrm{i}\partial_r\lambda^+ - \lambda^-\lambda^+ = -h^{-2}\xi^2 + \mathrm{i}h^{-1}\partial_s h^{-1}\xi - \tau. \end{aligned} \tag{5}$$

Considering the asymptotic expansions of the symbols, the rules of symbolic calculus and identifications of the $M$-quasi homogeneity in the class $S_M^2$, we immediately obtain the principal symbols: $\lambda_1^{\pm}(r, s, \tau, \xi) = \rho^{\pm}(r, s, \xi, \tau)$ in the $M$-quasi hyperbolic region. This last choice of $\lambda_1^+$ is directly linked to the characterization of the forward bicharacteristic.

Keeping on the different identifications in the classes of lower orders, we can conclude thanks to (5) that the symbols of the asymptotic expansion are given by the recursive relations:

$$\lambda_0^+(r, s, \tau, \xi) = \frac{1}{2\lambda_1^+}\big(\mathrm{i}h^{-1}\partial_s h^{-1}\xi + \mathrm{i}\partial_\xi\lambda_1^+\partial_s\lambda_1^+ - \mathrm{i}\partial_r\lambda_1^+ - \mathrm{i}\kappa_r\lambda_1^+\big) \tag{6}$$

and

$$\begin{aligned} \lambda_{-j}^+(r, s, \tau, \xi) = \frac{1}{2\lambda_1^+}\Bigg(&-\mathrm{i}\partial_r\lambda_{-j+1}^+ - \mathrm{i}\kappa_r\lambda_{-j+1}^+ - \sum_{l=0}^{j-1}\lambda_{-l}^+\lambda_{1-j+l}^+ \\ &- \sum_{\alpha=1}^{j+1}\frac{(-\mathrm{i})^\alpha}{\alpha!}\sum_{l=-1}^{j-\alpha}\partial_\xi^\alpha\lambda_{-l}^+\partial_s^\alpha\lambda_{1-j+l+\alpha}^+\Bigg), \end{aligned} \tag{7}$$

for all integers $j \geqslant 1$. The uniqueness of the asymptotic expansions of both $\lambda^+$ and $\lambda^-$ in $S_M^1$ follows from these relations. This ends the proof. □

*Remark* 3. – We might also write $L = (\partial_r + \mathrm{i}\hat{\Lambda}^+)(\partial_r + \mathrm{i}\hat{\Lambda}^-) + \hat{R}$. However, this factorization coupled to the theory of propagation of singularities [22,26] leads to control the incident wave.

Factorization (2) implies that the reflected part of the solution [22] is given by $v^+ = (\partial_{\mathbf{n}} + \mathrm{i}\Lambda^+)v$. The transparent condition, i.e. the nonreflecting boundary condition, of the solution $v$ at the boundary, is then set as:

$$v^+ \equiv T^+v \equiv \big(\partial_{\mathbf{n}} + \mathrm{i}\widetilde{\Lambda^+}\big)v = 0, \quad \text{on } \Sigma, \tag{8}$$

where the boundary pseudodifferential operator $\widetilde{\Lambda^+}$ is defined by $\widetilde{\Lambda^+} = \Lambda^+_{|_{r=0}}$.

## 3. Quasi-polynomial microlocal structure of the nonreflecting operator $T^+$

In fact, it is possible to refine the characterization of the expansion of $\lambda^+$ by precising its subjacent algebraic structure. To this end, introduce the subclass of $S_M^m$ of order $m$, denoted by $\mathbb{S}_M^m$, of quasi-polynomial symbols:

$$\mathbb{S}_M^m = \left\{a(r,s,\xi,\tau) \in S_M^m;\ \exists P^m \in \mathbb{P}_d \text{ such that } a(r,s,\xi,\tau) = \left(\lambda_1^+\right)^m P^m(r,s;X)\right\}, \quad m \in \mathbb{Z}.$$

Here, $\mathbb{P}_d$ stands for the space of polynomials of degree $d$ with $\mathcal{C}^\infty$ coefficients in $(r,s)$ and of symbolic variable of null inhomogeneity $X = \xi/\lambda_1^+$:

$$P^m(r,s;X) = \sum_{\gamma=0}^{d} p_\gamma^m(r,s) X^\gamma. \tag{9}$$

Let us now introduce the class of pseudodifferential operators whose symbol admits an asymptotic expansion in $\mathbb{S}_M^m$.

DEFINITION 2. – *A pseudodifferential operator $A$ of order $m$ is said to be in the class $OP\mathbb{S}_M^m$ if its symbol $a$ admits an asymptotic expansion of the form*:

$$a(r,s,\xi,\tau) \sim \sum_{j=-m}^{+\infty} a_{-j}(r,s,\xi,\tau),$$

*where each symbol $a_{-j}$ owns to $\mathbb{S}_M^{-j}$, $j \geqslant -m$.*

Now, let us derive some stability properties on the effect of a derivation with respect to a primal or dual variable on an element $a$ of the class $\mathbb{S}_M^m$.

PROPOSITION 2. – *Let $a \in \mathbb{S}_M^m$ be a quasi-polynomial symbol of order $m$, $m \in \mathbb{Z}$. Then, we have the following stability results by application of a derivation*:

$$\partial_\mu^\alpha a \in \mathbb{S}_M^m,\ \mu = r \text{ or } s, \quad \text{and} \quad \partial_\xi^\alpha a \in \mathbb{S}_M^{m-\alpha},\ \forall \alpha \in \mathbb{N}.$$

*Proof.* – The proof is based on the following equalities:

$$\begin{aligned} &\partial_\mu^\alpha X^\beta \in \mathbb{S}_M^0,\ \mu = r \text{ or } s, \quad \partial_\xi^\alpha X^\beta \in \mathbb{S}_M^{-\alpha}, \\ &\partial_\mu^\alpha \left(\lambda_1^+\right)^m \in \mathbb{S}_M^m,\ \mu = r \text{ or } s, \quad \partial_\xi^\alpha \left(\lambda_1^+\right)^m \in \mathbb{S}_M^{m-\alpha}, \end{aligned} \tag{10}$$

where both $m$ and $\gamma$ are some non-negative fixed integers. These results may, e.g., be obtained recursively on the order of derivation $\alpha$ and by a straightforward derivation.

Now, if we consider a symbol $a \in \mathbb{S}_M^m$, then we have by definition: $a = (\lambda_1^+)^m P^m(r,s;X)$. A derivation with respect to the primal variable $\mu$ shows that:

$$\partial_\mu^\alpha a = \sum_{\gamma=0}^{\alpha} C_\alpha^\gamma \partial_\mu^\gamma \left(\lambda_1^+\right)^m \partial_\mu^{\alpha-\gamma} P^m, \quad \mu = r \text{ or } s, \tag{11}$$

where $C_\alpha^\gamma$ is the Leibniz's coefficient and $P$ is of the form (9). As a consequence, we can assert that

$$\partial_\mu^{\alpha-\gamma} P^m = \sum_{\beta=0}^{d} \sum_{\delta=0}^{\alpha-\gamma} C_\delta^{\alpha-\gamma} \partial_\mu^\delta p_\beta^m \partial_\mu^{\alpha-\gamma-\delta} X^\beta.$$

From (10), we have the characterization $\partial_\mu^{\alpha-\gamma-\delta} X^\beta \in \mathbb{S}_M^0$. But since by hypothesis $\partial_\mu^\delta p_\beta^m$ is a $\mathcal{C}^\infty$ coefficient in $(r,s)$, we deduce that $\partial_\mu^{\alpha-\gamma} P^m$ is a linear combination of terms of $\mathbb{S}_M^0$ and so $\partial_\mu^{\alpha-\gamma} P^m \in \mathbb{S}_M^0$. Furthermore, (10) also gives us $\partial_\mu^\gamma (\lambda_1^+)^m \in \mathbb{S}_M^m$. This allows us to conclude that, since $\partial_\mu^\gamma (\lambda_1^+)^m \partial_\mu^{\alpha-\gamma} P^m \in \mathbb{S}_M^m$, a simple summation on (11) implies that $\partial_\mu^\alpha a \in \mathbb{S}_M^m$.

A similar analysis can be done for $\partial_\xi^\alpha a \in \mathbb{S}_M^{m-\alpha}$ and completes the proof. □

The introduction of this specific class of pseudodifferential operators allows to give a sharper algebraic description of the form of the operator $\Lambda^+$ as shown in the two following statements.

PROPOSITION 3. – *The terms $\lambda_{-j}^+$ defining the asymptotic expansion of $\lambda^+$ fulfill $\lambda_{-j}^+ \in \mathbb{S}_M^{-j}$, for every $j \geqslant -1$.*

*Proof.* – The proof can be obtained by some recursive arguments noticing that the result is obvious for $\lambda_1^+$.

Let us analyze relation (6) which expresses the $M$-quasi homogeneous term $\lambda_0^+$ of order zero. From the above derivation rules (10), we can directly assert that $\mathrm{i}\partial_\xi \lambda_1^+ \partial_s \lambda_1^+ \in \mathbb{S}_M^1$ and $\mathrm{i}\partial_r \lambda_1^+ \in \mathbb{S}_M^1$. Moreover, the following trivial properties are satisfied: $\mathrm{i}h^{-1}\partial_s h^{-1}\xi \in \mathbb{S}_M^1$ and $\mathrm{i}\kappa_r \lambda_1^+ \in \mathbb{S}_M^1$. From relation (10), the term $\lambda_0^+\lambda_1^+$ is in $\mathbb{S}_M^1$ which is equivalent to $\lambda_0^+ \in \mathbb{S}_M^0$.

Let us now assume that the characterization is fulfilled until the $(j-1)$-th order:

$$\forall l \text{ such that } -1 \leqslant l \leqslant j-1, \quad \lambda_{-l}^+ \in \mathbb{S}_M^{-l}.$$

Then from Proposition 2, the following relations hold by linear combinations:

$$-\sum_{\alpha=1}^{j+1} \frac{(-\mathrm{i})^\alpha}{\alpha!} \sum_{l=-1}^{j-\alpha} \partial_\xi^\alpha \lambda_{-l}^+ \partial_s^\alpha \lambda_{1-j+l}^+ \in \mathbb{S}_M^{1-j}, \qquad -\sum_{l=0}^{j-1} \lambda_{-l}^+ \lambda_{1-j+l}^+ \in \mathbb{S}_M^{1-j}$$

and

$$-\mathrm{i}\partial_r \lambda_{-j+1}^+ \in \mathbb{S}_M^{1-j}.$$

Moreover, we obviously have $-\mathrm{i}\kappa_r \lambda_{-j+1}^+ \in \mathbb{S}_M^{1-j}$. So, relation (7) implies that $\lambda_1^+\lambda_{-j}^+ \in \mathbb{S}_M^{1-j}$ and by division that $\lambda_{-j}^+ \in \mathbb{S}_M^{-j}$, ending hence the proof. □

THEOREM 4. – *The operator $\Lambda^+$ is a pseudodifferential operator of $\mathcal{C}^\infty(]-\varepsilon;\varepsilon[; OP\mathbb{S}_M^1)$. As a consequence, the boundary operator $\widetilde{\Lambda^+}$ on $\Sigma$ is an operator of $OP\mathbb{S}_M^1$.*

*Proof.* – The proof is simply a corollary of Proposition 3. □

## 4. Quasi-analytic characterizations of the symbol of $T^+$

### 4.1. Notations

To go further in the characterization of $\Lambda^+$, we now investigate the form of the polynomial part of each inhomogeneous symbol defining the asymptotic expansion. For the sake of brevity, we do not precise anymore the character $+$ which distinguishes the forward quantities from the backward ones. Therefore, operator $\Lambda^+$ is henceforth simply denoted by $\Lambda$.

Let us recall that, according to Proposition 3, each symbol $\lambda_{-j}$ can be written

$$\forall j \geqslant -1, \quad \lambda_{-j}(r,s,\tau,\xi) = (\lambda_1)^{-j} P^j(r,s;X), \tag{12}$$

where $P^j$ is a polynomial with $C^\infty$ coefficients in $(r,s)$:

$$P^j(r,s;X) = \sum_{\gamma=0}^{d(P^j)} p_\gamma^j(r,s) X^\gamma. \tag{13}$$

In the sequel, we precise the degree $d_j = d(P^j)$ and the coefficients $\{p_\gamma^j\}_{\gamma=0}^{d_j}$ involving in equation (13).

To this end, several notations are needed. Let $H$ be the Heaviside's function, i.e., the function such that $H(x) = 1$, if $x \geqslant 0$, and 0 otherwise. The brackets $[\cdot]$ stand for the low integer part of a non-negative real number. Let us introduce the following sequences of indices:

$$\begin{aligned}
&a_j = j + \left[\frac{j}{2}\right] + 1 + \left(j - 2\left[\frac{j}{2}\right]\right), && \tilde{a}_j = j + \left[\frac{j}{2}\right] + 1,\\
&b_{j,k} = 2(k-1-j)H\big(k-(j+2)\big), && \tilde{b}_{j,k} = \big(2(k-j)-1\big)H\big(k-(j+1)\big),\\
&c_j = j + \left(j - 2\left[\frac{j}{2}\right]\right), && \tilde{c}_j = j + \left(j+1-2\left[\frac{j+1}{2}\right]\right),
\end{aligned}$$

where $k$ and $j$ are in $\mathbb{N}$ (notation $(j - [j/2])$ only indicates the parity of $j$). It is seen later (Lemma 8) that these indices can in fact be very easily rewritten thanks to the parity of $j$. We can immediately remark that the following equalities hold $b_{j,a_j} = c_j$ and $\tilde{b}_{j,\tilde{a}_j} = \tilde{c}_j$.

Now, consider a non-negative integer $p$ and a multiindex $\beta \in \mathbb{N}^{p+1}$ such that $\beta = (\beta^0, \ldots, \beta^p)$. We can then define the inner product of two multiindices $\alpha$ and $\beta$ by: $\alpha \cdot \beta = \sum_{j=0}^p \alpha^j \beta^j$. The associated length $|\cdot|$ of a multiindex $\beta$ is set to: $|\beta| = 1 \cdot \beta$. Then, let us now introduce the following set of multiindices which will play an important role:

$$E_j = \big\{\beta \in \mathbb{N}^{j+1} \mid \alpha = (0,1,\ldots,j) \text{ and } \alpha\cdot\beta \leqslant j, |\beta| \leqslant j\big\}.$$

We designate by $j^\#$ the cardinal number of $E_j$.

Some vectorial and matricial notations are also required. Let $k$ and $\rho$ be two non-negative integers satisfying conditions $0 \leqslant k \leqslant a_j$ and $b_{j,k} \leqslant \rho \leqslant c_j$. Let $C_{k,\rho} \in \mathbb{Q}^{(j+1)^\#}$ be a vector whose $(j+1)^\#$ components are rational coefficients and $\delta_{k,\rho} = (\delta_l(k,\rho))_{1 \leqslant l \leqslant (j+1)^\#}$ a vector with some row-vectors of $\mathbb{N}^{j+2}$ as components. Thus, the vector of exponents $\delta_{k,\rho}$ can be identified to a matrix of integers of $\mathcal{M}_{(j+1)^\#, j+2}(\mathbb{N})$ as follows:

$$\delta_{k,\rho} \equiv \begin{pmatrix}
\delta_1^{(0)}(k,\rho) & \delta_1^{(1)}(k,\rho) & \cdots & \delta_1^{(j+1)}(k,\rho)\\
\delta_2^{(0)}(k,\rho) & \delta_2^{(1)}(k,\rho) & \cdots & \delta_2^{(j+1)}(k,\rho)\\
\vdots & & & \vdots\\
\delta_{(j+1)^\#}^{(0)}(k,\rho) & \delta_{(j+1)^\#}^{(1)}(k,\rho) & \cdots & \delta_{(j+1)^\#}^{(j+1)}(k,\rho)
\end{pmatrix}.$$

If for $1 \leqslant l \leqslant (j+1)^\#$ vectors $\delta_l(k,\rho)$ are some elements of $E_{j+1}$, we then will adopt the notation: $\delta_{k,\rho} \in \mathbb{E}_{j+1}$. Furthermore, if these exponents also fulfill $\delta_l(k,\rho) \neq (\delta_l^{(0)}(k,\rho), 0, \ldots, 0)$, with $\delta_l^{(0)}(k,\rho) \leqslant j+1$, for every $l \in \{1,\ldots,(j+1)^{\#}\}$, it is quoted $\delta_{k,\rho} \in \mathbb{E}_{j+1}^{*}$. If there exists $l \in \{1,\ldots,(j+1)^{\#}\}$ such that $\delta_l(k,\rho) = (j+1,0,\ldots,0)$, it is noticed $\delta_{k,\rho} \in \tilde{\mathbb{E}}_{j+1}$. Similarly, we define the array $\mathbb{I}_{j+1}$ with $(j+1)$ columns and $(j+1)^{\#}$ rows such that:

$$\mathbb{I}_{j+1} \equiv \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ 1 & 0 & \cdots & 0 \end{pmatrix}.$$

Now, let us introduce the vector $D^{(j+1)}(\kappa) \in (\mathcal{C}^{\infty}(\Gamma))^{j+2}$ of derivatives of the curvature $\kappa$: $D^{(j+1)}(\kappa) = (d_s^l \kappa)_{0 \leqslant l \leqslant j+1}$. This allows us to define the element $D^{(j+1)}(\kappa)^{\delta_{k,\rho}}$ of $\mathcal{M}_{(j+1)\#,j+2}(\mathcal{C}^{\infty}(\Gamma))$ by:

$$D^{(j+1)}(\kappa)^{\delta_{k,\rho}} = \begin{pmatrix} \kappa^{\delta_1^{(0)}(k,\rho)} & (d_s\kappa)^{\delta_1^{(1)}(k,\rho)} & \cdots & (d_s^{j+1}\kappa)^{\delta_1^{(j+1)}(k,\rho)} \\ \kappa^{\delta_2^{(0)}(k,\rho)} & (d_s\kappa)^{\delta_2^{(1)}(k,\rho)} & \cdots & (d_s^{j+1}\kappa)^{\delta_2^{(j+1)}(k,\rho)} \\ \vdots & & & \vdots \\ \kappa^{\delta^{(0)}_{(j+1)^{\#}}(k,\rho)} & (d_s\kappa)^{\delta^{(1)}_{(j+1)^{\#}}(k,\rho)} & \cdots & (d_s^{j+1}\kappa)^{\delta^{(j+1)}_{(j+1)^{\#}}(k,\rho)} \end{pmatrix} \tag{14}$$

for $\delta_{k,\rho} \in \mathbb{E}_{j+1}$. Let us set as $D^{(j+1)}(\kappa)^{\otimes\delta_{k,\rho}} \in (\mathcal{C}^{\infty}(\Gamma))^{(j+1)^{\#}}$ the compressed vector whose components are some products of the coefficients for a given row, that is

$$D^{(j+1)}(\kappa)^{\otimes\delta_{k,\rho}} = \left( \prod_{l=0}^{j+1} \left(d_s^l \kappa\right)^{\delta_p^{(l)}(k,\rho)} \right)_{1 \leqslant p \leqslant (j+1)^{\#}}.$$

Moreover, if we suppose that the degrees $\delta_{k,\rho}$ are some elements of $\mathbb{E}_{j+1}$ and that $C_{k,\rho} \in \mathbb{Q}^{(j+1)^{\#}}$, we can define the following quantity:

$$\left\langle C_{k,\rho}, D^{(j+1)}(\kappa)^{\otimes\delta_{k,\rho}} \right\rangle_{(j+1)^{\#}}. \tag{15}$$

So, this last relation precises that this term is a linear combination of products of powers (of $E_j$) of derivatives of the curvature. Hence we can define a matrix $A = (A_{k,\rho})_{0 \leqslant k \leqslant a_j, 0 \leqslant \rho \leqslant c_j}$ of $\mathcal{M}_{a_j+1,c_j+1}(\mathcal{C}^{\infty}(\Gamma))$ of the form:

$$\begin{array}{cc} 0 & \longrightarrow \\ 1 & \longrightarrow \\ \vdots & \vdots \\ j+1 & \longrightarrow \\ j+2 & \longrightarrow \\ j+3 & \longrightarrow \\ \vdots & \vdots \\ a_j & \longrightarrow \end{array} \begin{pmatrix} A_{0,0} & A_{0,1} & A_{0,2} & A_{0,3} & A_{0,4} & \cdots & A_{0,c_j} \\ A_{1,0} & A_{1,1} & A_{1,2} & A_{1,3} & A_{1,4} & \cdots & A_{1,c_j} \\ \vdots & & & & \vdots & & \\ A_{j+1,0} & A_{j+1,1} & A_{j+1,2} & A_{j+1,3} & A_{j+1,4} & \cdots & A_{j+1,c_j} \\ 0 & 0 & A_{j+2,2} & A_{j+2,3} & A_{j+2,4} & \cdots & A_{j+2,c_j} \\ 0 & 0 & 0 & 0 & A_{j+3,4} & \cdots & A_{j+3,c_j} \\ \vdots & & & & \vdots & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & A_{a_j,c_j} \end{pmatrix},$$

where the components $A_{k,\rho}$ are defined by equation (15). This writting is valid since $c_j$ is, by definition, always even. Null coefficients begin to appear from the row $l = j+2$ according to the definition of $b_{j,k}$ for some column indices varying until $2(l-j-1)$.

Similarly, we introduce a matrix $B = (B_{k,\rho})_{0\leqslant k\leqslant \tilde{a}_j, 0\leqslant \rho\leqslant \tilde{c}_j}$ which can be rewritten (since $\tilde{c}_j$ is always odd):

$$\begin{array}{cc} 0 & \longrightarrow \\ 1 & \longrightarrow \\ \vdots & \vdots \\ j+1 & \longrightarrow \\ j+2 & \longrightarrow \\ j+3 & \longrightarrow \\ \vdots & \vdots \\ \tilde{a}_j & \longrightarrow \end{array}
\begin{pmatrix} B_{0,0} & B_{0,1} & B_{0,2} & B_{0,3} & B_{0,4} & \cdots & B_{0,\tilde{c}_j} \\ B_{1,0} & B_{1,1} & B_{1,2} & B_{1,3} & B_{1,4} & \cdots & B_{1,\tilde{c}_j} \\ \vdots & & & & \vdots & & \\ 0 & B_{j+1,1} & B_{j+1,2} & B_{j+1,3} & B_{j+1,4} & \cdots & B_{j+1,\tilde{c}_j} \\ 0 & 0 & 0 & B_{j+2,3} & B_{j+2,4} & \cdots & B_{j+2,\tilde{c}_j} \\ 0 & 0 & 0 & 0 & 0 & \cdots & B_{j+3,\tilde{c}_j} \\ \vdots & & & & \vdots & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & B_{\tilde{a}_j,\tilde{c}_j} \end{pmatrix}.$$

Until the end of the paper, the exponents e and o respectively designate the even and odd terms.

### 4.2. Characterization results

These notations being ended, we can announce the quasi-analytic characterization result about the asymptotic expansion of the transparent operator near the boundary $\Gamma_r$.

THEOREM 5. – *Let $j \in \mathbb{N}$. We consider the indices $k \in \{0,\dots,a_j\}$, $\rho \in \{b_{j,k},\dots,c_j\}$, $\tilde{k} \in \{0,\dots,\tilde{a}_j\}$ and $\tilde{\rho} \in \{\tilde{b}_{j,k},\dots,\tilde{c}_j\}$. Then, there exist some pairs of exponents $(\delta^{\mathrm{e}}_{k,\rho}, \delta^{\mathrm{o}}_{\tilde{k},\tilde{\rho}}) \in \tilde{\mathbb{E}}_{j+1} \times \mathbb{E}^*_{j+1}$ and some pairs of rational coefficients $(C^{\mathrm{e}}_{k,\rho}, C^{\mathrm{o}}_{\tilde{k},\tilde{\rho}})$ of $\mathbb{Q}^{(j+1)^\#} \times \mathbb{Q}^{(j+1)^\#}$ such that*:

$$\lambda_{-j} = (\lambda_1)^{-j}(i)^{j+3}\big(h^{-1}\big)^{j+1}\Bigg\{\sum_{k=0}^{a_j}\Bigg[\sum_{\rho=0}^{c_j} A_{k,\rho}\big(h^{-1}r\big)^{\rho}\Bigg]\big(h^{-1}X\big)^{2k} + \sum_{\tilde{k}=0}^{\tilde{a}_j}\Bigg[\sum_{\tilde{\rho}=0}^{\tilde{c}_j} B_{\tilde{k},\tilde{\rho}}\big(h^{-1}r\big)^{\tilde{\rho}}\Bigg]\big(h^{-1}X\big)^{2\tilde{k}+1}\Bigg\}. \tag{16}$$

*Another equivalent expression is given by*:

$$\begin{aligned}\lambda_{-j} &= (\lambda_1)^{-j}(i)^{j+3}(h^{-1})^{j+1} \\ &\quad\times\Bigg\{\sum_{k=0}^{a_j}\Bigg[\sum_{\rho=b_{j,k}}^{c_j}\big\langle C^{\mathrm{e}}_{k,\rho}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{k,\rho}}\big\rangle_{(j+1)^\#}\big(h^{-1}r\big)^{\rho}\Bigg]\big(h^{-1}X\big)^{2k} \\ &\qquad + \sum_{\tilde{k}=0}^{\tilde{a}_j}\Bigg[\sum_{\tilde{\rho}=\tilde{b}_{j,k}}^{\tilde{c}_j}\big\langle C^{\mathrm{o}}_{\tilde{k},\tilde{\rho}}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{o}}_{\tilde{k},\tilde{\rho}}}\big\rangle_{(j+1)^\#}\big(h^{-1}r\big)^{\tilde{\rho}}\Bigg]\big(h^{-1}X\big)^{2\tilde{k}+1}\Bigg\}.\end{aligned} \tag{17}$$

*Remark* 4. – The higher-order term according to $X$ in (16) is $(h^{-1}X)^{3(j+1)}$, for every integer $j \geqslant 0$. Thus, the degree of the polynomial is given by: $d(P^j) = 3(j+1)$. Moreover, since $\delta^{\mathrm{o}}_{k,\rho} \in \mathbb{E}^*_{j+1}$, the odd terms always include at least one term of derivative of the curvature. This is an essential point since for a constant curvature only the even terms keep on.

Before proving Theorem 5, we give two other characterization results. More precisely, the above theorem yields a detailed form of the microlocal asymptotic expansion of the operator $\Lambda$.

However, the interesting operator is rather the boundary operator $\tilde{\Lambda}$. A direct consequence of Theorem 5 for $r = 0$ is given by the following statement:

THEOREM 6. – *Under the notations of Theorem* 5*, the asymptotic expansion of the symbol of the operator* $\widetilde{\Lambda} = \Lambda_{|r=0}$ *is given by*:

$$\begin{aligned} &\widetilde{\lambda_1} = -\big(-\big(\xi^2 + \tau\big)\big)^{1/2}, \\ &\widetilde{\lambda_{-j}} = (\widetilde{\lambda_1})^{-j}(\mathrm{i})^{j+3}\left\{\sum_{k=0}^{j+1} A_k X^{2k} + \sum_{k=0}^{j} B_k X^{2k+1}\right\}, \quad j \geqslant 0, \end{aligned} \tag{18}$$

*where coefficients* $A_k$ *and* $B_k$ *are some linear combinations of products of powers of derivatives of the curvature. More precisely, we get*

$$A_k = \big\langle C_k^{\mathrm{e}}, D^{(j+1)}(\kappa)^{\otimes \delta_k^{\mathrm{e}}}\big\rangle_{(j+1)^\#}, \qquad B_k = \big\langle C_k^{\mathrm{o}}, D^{(j+1)}(\kappa)^{\otimes \delta_k^{\mathrm{o}}}\big\rangle_{(j+1)^\#}, \tag{19}$$

*where* $(C_k^{\mathrm{e}}, C_k^{\mathrm{o}}) \in \mathbb{Q}^{(j+1)^\#} \times \mathbb{Q}^{(j+1)^\#}$ *and* $(\delta_k^{\mathrm{e}}, \delta_k^{\mathrm{o}}) \in \tilde{\mathbb{E}}_{j+1} \times \mathbb{E}_{j+1}^*$*, for every* $k$ *in* $\{0, \dots, j+1\}$ *or* $\{0, \dots, j\}$ *thanks to the parity of the considered term.*

*Proof.* – The proof is immediate from the previous theorem. Indeed, set $r = 0$ in equation (16) for the even term. Then, since $b_{j,k} = 0$ if $k$ is equal to or lower than $(j+1)$, the greater terms vanish because of the nullity of $(h^{-1}r)^\rho$. So, we get the even part appearing in the proposition. A similar proof gives the result for the odd part. □

At this step, several remarks must be done. In the case of a null curvature, each term $\widetilde{\lambda_{-j}}$, $j \geqslant 0$, vanishes and the transparent operator in [9] is obviously recovered. Moreover, it is noticeable that the choice of the subalgebra of pseudodifferential operators in which the transparent operator is described is only conditioned by the principal symbol $\lambda_1$. Thus these characterizations also hold for the wave or heat scalar operators only choosing the appropriate class of operators. Moreover, Theorems 5 and 6 may be extended to equations in higher dimensions using some similar calculations as in [3] for the three-dimensional case and in [23] for greater dimensions. Finally, the possible presence of a space dependent potential in the Schrödinger equation does not really affect the previous analysis.

In the case where the curvature is locally constant, the following corollary occurs:

COROLLARY 7. – *If the curvature is locally constant, symbols* $(\widetilde{\lambda_{-j}})_{j \geqslant -1}$ *are given by*:

$$\widetilde{\lambda_1} = -\big(-\big(\xi^2 + \tau\big)\big)^{1/2} \quad \textit{and} \quad \widetilde{\lambda_{-j}} = -(\widetilde{\lambda_1})^{-j}(\mathrm{i}\kappa)^{j+1}\sum_{k=0}^{j+1} c_k X^{2k}, \quad \textit{for } j \geqslant 0,$$

*with* $c_k \in \mathbb{Q}$.

*Proof.* – The result is a consequence of the property on the exponents: $(\delta_k^{\mathrm{e}}, \delta_k^{\mathrm{o}}) \in \tilde{\mathbb{E}}_{j+1} \times \mathbb{E}_{j+1}^*$ and of Remark 4. Indeed, the exponents $\delta_k^{\mathrm{e}}$ are such that there exists $l \in \{1, \dots, (j+1)^\#\}$ satisfying $\delta_{k,l}^{\mathrm{e}} = (j+1, 0, \dots, 0)$. Furthermore, the characterization of $\delta_k^{\mathrm{o}} \in \mathbb{E}_{j+1}^*$ indicates that each function depending on $s$ factor of an odd polynomial in $h^{-1}X$ is a product of derivatives of the curvature and so vanishes in our particular case. □

All these properties can be immediately observed on the three symbols $\lambda_1$, $\lambda_0$ and $\lambda_{-1}$ as seen below.

### 4.3. Initialization of the proof and two examples

To establish Theorem 5, we recall the characterization of each symbol $\lambda_{-j}^{+}$ obtained during the proof of Theorem 1, i.e.:

$$\lambda_0(r,s,\tau,\xi) = \frac{1}{2\lambda_1}\left(\mathrm{i}h^{-1}\partial_s h^{-1}\xi + \mathrm{i}\partial_\xi\lambda_1\partial_s\lambda_1 - \mathrm{i}\partial_r\lambda_1 - \mathrm{i}\kappa_r\lambda_1\right)$$

and, for $j \geqslant 1$,

$$\begin{aligned}\lambda_{-j} = \frac{1}{2\lambda_1}\Bigg\{ & -\mathrm{i}\partial_r\lambda_{-j+1} - \mathrm{i}\kappa_r\lambda_{-j+1} - \sum_{l=0}^{j-1}\lambda_{-l}\lambda_{1-j+l} \\ & - \sum_{\alpha=1}^{j+1}\frac{(-\mathrm{i})^\alpha}{\alpha!}\sum_{l=-1}^{j-\alpha}\partial_\xi^\alpha\lambda_{-l}\partial_s^\alpha\lambda_{1-j+l+\alpha}\Bigg\}.\end{aligned} \tag{20}$$

We use a recursive approach based on the above formulas to demonstrate Theorem 5. To clarify the exposure of the proof, we split it into several parts, each of them being devoted to one term of the previous expression.

The initialization step consists to precise the case of symbol $\lambda_0$. Furthermore, to illustrate the two characterization results, we also explain in details their meaning on symbol $\lambda_{-1}$ (which is computed by using the above relations implemented in a computer algebra system).

**Symbols $\lambda_0$ and $\tilde{\lambda}_0$: initialization step.** Let us consider symbol $\lambda_0$:

$$\lambda_0 = (\lambda_1)^0(\mathrm{i})^3h^{-1}\left\{\frac{1}{2}\partial_s\kappa\left(rh^{-1}\right)\left(h^{-1}X\right)^3 - \frac{1}{2}\kappa\left(h^{-1}X\right)^2 + \frac{1}{2}\partial_s\kappa\left(rh^{-1}\right)\left(h^{-1}X\right) - \frac{1}{2}\kappa\left(h^{-1}X\right)^0\right\}.$$

This expression is consistent with (16)–(17). Indeed, we can easily check that: $a_0 = 1$, $b_{0,k} = 2(k-1)H(k-2)$, $c_0 = 0$, $\tilde{a}_0 = 1$, $\tilde{b}_{0,k} = (2k-1)H(k-1)$ and $\tilde{c}_0 = 1$. Hence, there are two even monomials: $X^2$ and 1, and two odd ones: $X^3$ and $X$. Moreover, a direct calculation yields: $1^\# = 3$, $\tilde{\mathbb{E}}_1 = \{(1,0)\}$ and $\mathbb{E}_1^* = \{(0,1)\}$, which traduces that only the terms in $\kappa$ appear in front of the even parts and the terms in $\partial_s\kappa$ are some coefficients of the odd terms. In the even case, $\rho$ always vanishes and so there is no term in $(h^{-1}r)^\rho$. This is no more the case for the odd part since $\rho = 0$ or 1 implies the existence of non-vanishing terms $h^{-1}r$ in the odd coefficients. Setting $r = 0$ in the above expression, we obtain on the boundary $\Gamma$:

$$\tilde{\lambda}_0 = (\mathrm{i})^3\left\{-\frac{1}{2}\kappa X^2 - \frac{1}{2}\kappa\right\},$$

since $h^{-1} = 1$. This relation is in accordance with (18)–(19) with regards to the preceding results and remarks.

**Symbols $\lambda_{-1}$ and $\tilde{\lambda}_{-1}$.** The symbol of order $-1$ is set to:

$$\begin{aligned}\lambda_{-1} = \lambda_1^{-1}h^{-2}(\mathrm{i})^4\Bigg\{ & \frac{15}{8}(\partial_s\kappa)^2\left(h^{-1}r\right)^2\left(h^{-1}X\right)^6 + \frac{1}{2}\kappa\,\partial_s\kappa\left(rh^{-1}\right)\left(h^{-1}X\right)^5 \\ & + \left(\frac{15}{4}(\partial_s\kappa)^2\left(h^{-1}r\right)^2 - \frac{1}{2}\partial_s^2\kappa\left(h^{-1}r\right) - \frac{3}{8}\kappa^2\right)\left(h^{-1}X\right)^4 + \frac{1}{2}\kappa\,\partial_s\kappa\left(h^{-1}r\right)\left(h^{-1}X\right)^3 \\ & + \left(\frac{15}{8}(\partial_s\kappa)^2\left(h^{-1}r\right)^2 - \frac{1}{2}\partial_s^2\kappa\left(h^{-1}r\right) - \frac{1}{4}\kappa^2\right)\left(h^{-1}X\right)^2 - \frac{1}{4}\kappa\,\partial_s\kappa\left(h^{-1}r\right)\left(h^{-1}X\right) + \frac{3}{8}\kappa\Bigg\},\end{aligned}$$

and is of the expected form. The bounds in which vary the indices $k$ and $\rho$ are: $a_1 = 3$, $b_{1,k} = 2(k-2)H(k-3)$, $c_1 = 2$, $\tilde{a}_1 = 2$, $\tilde{b}_{1,k} = (2(k-1)-1)H(k-2)$ and $\tilde{c}_1 = 1$. The dominating degree of the polynomial with respect to $h^{-1}X$ is 6. As a consequence, the index $\rho$ associated with the even terms is included between 0 and 2 except for $k = 3$ where its value is equal to 2. The set $E_2$ is such that: $E_2 = \{(0,0,0), (0,1,0), (0,0,1), (0,2,0), (1,0,0), (1,1,0), (1,0,1), (2,0,0)\}$, and so $2^{\#} = 8$. This shows that some terms with only $\kappa^2$ in front of an even term can exist conversely to the odd case where there is always at least one derivative $\partial_s\kappa$ or $\partial_s^2\kappa$ with a non-vanishing exponent (description contained in the set $\mathbb{E}_2^*$). The expression of this symbol on the boundary $\Gamma$ is:

$$\tilde{\lambda}_{-1} = \lambda_1^{-1}(\mathrm{i})^4\left\{-\frac{3}{8}\kappa^2X^4 - \frac{1}{4}\kappa^2X^2 + \frac{3}{8}\kappa^2\right\}.$$

According to (18)–(19), we easily see that the degree of the polynomial in $X$ is equal to 4. Finally, symbol $\tilde{\lambda}_{-1}$ possesses the suggested structure.

### 4.4. Characterization of the two first terms of expression (20)

We begin to consider the two first terms of (20) which can be analyzed in a very similar way.

PROPOSITION 1. – *Both terms* $-\mathrm{i}\partial_r\lambda_{-j+1}/(2\lambda_1)$ *and* $-\mathrm{i}\kappa_r\lambda_{-j+1}/(2\lambda_1)$ *are of the form* (16)–(17) *for some exponents* $(\delta^{\mathrm{e}}_{k,\rho}, \delta^{\mathrm{o}}_{k,\rho})$ *of* $\tilde{\mathbb{E}}_{j+1} \times \mathbb{E}^*_{j+1}$ *and suitable pairs of rational coefficients* $(C^{\mathrm{e}}_{k,\rho}, C^{\mathrm{o}}_{k,\rho})$ *of* $\mathbb{Q}^{(j+1)\#} \times \mathbb{Q}^{(j+1)\#}$.

*Proof.* – The recursivity assumption leads us to assume that, for a fixed integer $j$, term $\lambda_{-j+1}$ can be written as:

$$\lambda_{-j+1} = (\mathrm{i})^{j+2}\lambda_1^{-j+1}\left(h^{-1}\right)^j P(X),$$

where polynomial $P$ is defined by:

$$\begin{aligned} P(X) = &\sum_{k=0}^{a_{j-1}}\sum_{\rho=b_{j-1,k}}^{c_{j-1}}\left(\left\langle C^{\mathrm{e}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{k,\rho}}\right\rangle_{j^\#}\left(h^{-1}r\right)^\rho\right)\left(h^{-1}X\right)^{2k} \\ &+ \sum_{k=0}^{\tilde{a}_{j-1}}\sum_{\rho=\tilde{b}_{j-1,k}}^{\tilde{c}_{j-1}}\left(\left\langle C^{\mathrm{o}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes\delta^{\mathrm{o}}_{k,\rho}}\right\rangle_{j^\#}\left(h^{-1}r\right)^\rho\right)\left(h^{-1}X\right)^{2k+1}. \end{aligned}$$

Now, some straightforward derivations yield the following expressions:

$$\begin{aligned} &\partial_r\left(\lambda_1^{-j+1}\right) = -(j-1)\kappa h^{-3}X^2\lambda_1^{-j+1}, \\ &\partial_r\left(h^{-1}\right)^j = -j\left(h^{-1}\right)^{j+1}\kappa, \\ &\partial_r\left(h^{-1}r\right)^\rho = \begin{cases} \rho\left(h^{-1}r\right)^{\rho-1}h^{-1}\left(1-(h^{-1}r)\kappa\right), & \text{if } \rho > 1, \\ 0, \quad \text{otherwise}, \end{cases} \\ &\partial_r\left(h^{-1}X\right)^{2k} = -2kh^{-1}\kappa\left(h^{-1}X\right)^{2k}\left(1+h^{-2}X^2\right). \end{aligned}$$

By using these relations and deriving $\lambda_{-j+1}$ with respect to $r$, we get:

$$\partial_r\lambda_{-j+1} = (\mathrm{i})^{j+2}\lambda_1^{-j+1}\left(h^{-1}\right)^j\left\{-\kappa h^{-1}\left((j-1)h^{-2}X^2 + j\right)P(X) + \partial_r P(X)\right\}.$$

It is easy to see that the contribution of the part linked to $P$ is of the desired form. Now, compute polynomial $\partial_r P(X)$ given by:

$$\begin{aligned}
\partial_r P(X) &= \sum_{k=0}^{a_{j-1}} \sum_{\rho=b_{j-1,k}}^{c_{j-1}} \left( \left\langle C^{\mathrm{e}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \right\rangle_{j^\#} \partial_r \left(h^{-1} r\right)^{\rho} \right) \left(h^{-1} X\right)^{2k} \\
&\quad + \sum_{k=0}^{a_{j-1}} \sum_{\rho=b_{j-1,k}}^{c_{j-1}} \left( \left\langle C^{\mathrm{e}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \right\rangle_{j^\#} \left(h^{-1} r\right)^{\rho} \right) \partial_r \left(h^{-1} X\right)^{2k} \\
&\quad + \sum_{k=0}^{\tilde{a}_{j-1}} \sum_{\rho=\tilde{b}_{j-1,k}}^{\tilde{c}_{j-1}} \left( \left\langle C^{\mathrm{o}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{o}}_{k,\rho}} \right\rangle_{j^\#} \partial_r \left(h^{-1} r\right)^{\rho} \right) \left(h^{-1} X\right)^{2k+1} \\
&\quad + \sum_{k=0}^{\tilde{a}_{j-1}} \sum_{\rho=\tilde{b}_{j-1,k}}^{\tilde{c}_{j-1}} \left( \left\langle C^{\mathrm{o}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{o}}_{k,\rho}} \right\rangle_{j^\#} \left(h^{-1} r\right)^{\rho} \right) \partial_r \left(h^{-1} X\right)^{2k+1} \\
&= A + B + C + D,
\end{aligned}$$

where quantities $A$, $B$, $C$ and $D$ designate each of the sum appearing above. By the preceding relations, $A$ may be rewritten as:

$$\begin{aligned}
A &= h^{-1} \left( \sum_{k=0}^{a_{j-1}} \sum_{\substack{\rho=b_{j-1,k} \\ \rho>1}}^{c_{j-1}} \left( \left\langle \tilde{C}^{\mathrm{e}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \right\rangle_{j^\#} \left(h^{-1} r\right)^{\rho-1} \right) \left(h^{-1} X\right)^{2k} \right) \\
&\quad - h^{-1} \left( \sum_{k=0}^{a_{j-1}} \sum_{\substack{\rho=b_{j-1,k} \\ \rho>1}}^{c_{j-1}} \left( \kappa \left\langle \tilde{C}^{\mathrm{e}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \right\rangle_{j^\#} \left(h^{-1} r\right)^{\rho} \right) \left(h^{-1} X\right)^{2k} \right) \\
&= A_1 + A_2,
\end{aligned}$$

where $A_1$ and $A_2$ stand for each of the quantities in brackets in the previous expression and $\tilde{C}^{\mathrm{e}}_{k,\rho}$ are some constants of $\mathbb{Q}^{j^\#}$. By the change of index $R = \rho - 1$, we obtain

$$A_1 = h^{-1} \sum_{k=0}^{a_{j-1}} \sum_{R=b_{j,k}}^{c_{j-1}-1} \left( \left\langle \tilde{C}^{\mathrm{e}}_{k,R}, D^{(j)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,R}} \right\rangle_{j^\#} \left(h^{-1} r\right)^{R} \right) \left(h^{-1} X\right)^{2k}.$$

Finally, noticing that $c_{j-1} - 1 \leqslant c_j$, we see that $A_1$ has the desired structure. Let us now focus our attention on $A_2$. We have:

$$A_2 = -h^{-1} \sum_{k=0}^{a_{j-1}} \sum_{\rho=\max(b_{j-1,k},1)}^{c_{j-1}} \left( \left\langle \tilde{C}^{\mathrm{e}}_{k,\rho}, D^{(j)}(\kappa)^{\otimes \delta'^{\mathrm{e}}_{k,\rho}} \right\rangle_{j^\#} \left(h^{-1} r\right)^{\rho} \right) \left(h^{-1} X\right)^{2k},$$

where we set $\delta'^{\mathrm{e}}_{k,\rho} = \mathbb{I}_j + \delta^{\mathrm{e}}_{k,\rho}$. Since $\max(b_{j-1,k}, 1) > 0$, $A_2$ has the expected form. The treatment of $B$ is realized by factorizing $h^{-1}$ as above and next including the curvature $\kappa$ as for $A_2$. Quantity $(1 + h^{-2} X^2)$ implies that the upper bound of summation on $k$ is equal to $(a_{j-1} + 1)$ which is lower than $a_j$. Hence, we can conclude that $B$ falls within the scope of the general formula even if it means that we have to add some vanishing contants $C^{\mathrm{e}}_{k,\rho}$ and exponents $\delta^{\mathrm{e}}_{k,\rho}$ to be consistent with the inner product $\langle \cdot, \cdot \rangle_{(j+1)^\#}$. Both terms $C$ and $D$ are very similarly handled. Dividing by $\lambda_1$ and multiplying by i, the resulting quantity $-\mathrm{i}\partial_r \lambda_{-j+1}/(2\lambda_1)$ has the suggested form. To conclude the proof, we remark that only $A$ and $B$ contribute to $\delta^{\mathrm{e}}_{k,0} \in \tilde{\mathbb{E}}_{j+1}$.

To proof the result on $-\mathrm{i}\kappa_r\lambda_{-j+1}/(2\lambda_1)$, we develop it according to the parallel curvature $\kappa_r = h^{-1}\kappa$ and we adapt the previous approach. Exactly as above, it participates to $\delta^{\mathrm{e}}_{k,0} \in \tilde{\mathbb{E}}_{j+1}$. □

### 4.5. Product term without derivative in expression (20)

We consider now the third term of equation (20). More precisely, from the recursive assumption about symbols $\{\lambda_{-l}\}_{l=0}^{j-1}$, we get the following statement.

PROPOSITION 2. – *We have the relation*:

$$-\sum_{l=0}^{j-1}\frac{\lambda_{-l}\lambda_{1-j+l}}{2\lambda_1} = (\mathrm{i})^{j+3}\lambda_1^{-j}\big(h^{-1}\big)^{j+1}$$
$$\times\Bigg\{\sum_{k=0}^{a_j}\sum_{\rho=b_{j,k}}^{c_j}\big(\big\langle C^{\mathrm{e}}_{k,\rho}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{k,\rho}}\big\rangle_{(j+1)^{\#}}\big(h^{-1}r\big)^{\rho}\big)\big(h^{-1}X\big)^{2k}$$
$$+\sum_{k=0}^{\tilde a_j}\sum_{\rho=\tilde b_{j,k}}^{\tilde c_j}\big(\big\langle C^{\mathrm{o}}_{k,\rho}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{o}}_{k,\rho}}\big\rangle_{(j+1)^{\#}}\big(h^{-1}r\big)^{\rho}\big)\big(h^{-1}X\big)^{2k+1}\Bigg\},$$

*for some rational coefficients $C^{\mathrm{e,o}}_{k,\rho} \in \mathbb{Q}^{(j+1)^{\#}}$ and exponents $\delta^{\mathrm{e,o}}_{k,\rho}$ checking the assumptions of Theorem* 5.

*Proof.* – Let us recall that by the recursive hypothesis, $\forall l \in \{0,\dots,j-1\}$, we have:

$$\lambda_{-l} = (\mathrm{i})^{l+3}\lambda_1^{-l}\big(h^{-1}\big)^{l+1}\big\{P^{\mathrm{e}}_{-l}(X) + P^{\mathrm{o}}_{-l}(X)\big\},$$

where polynomials $P^{\mathrm{e}}_{-l}$ and $P^{\mathrm{o}}_{-l}$ are such that:

$$P^{\mathrm{e}}_{-l}(X) = \sum_{k=0}^{a_l}\left(\sum_{\rho=b_{l,k}}^{c_l} A^{\mathrm{e}}_{k,\rho}\big(h^{-1}r\big)^{\rho}\right)\big(h^{-1}X\big)^{2k} = \sum_{k=0}^{a_l}\mathcal{C}^{\mathrm{e}}_{k,l}(r,s)\big(h^{-1}X\big)^{2k},$$
$$P^{\mathrm{o}}_{-l}(X) = \sum_{k=0}^{\tilde a_l}\left(\sum_{\rho=\tilde b_{l,k}}^{\tilde c_l} B^{\mathrm{o}}_{k,\rho}\big(h^{-1}r\big)^{\rho}\right)\big(h^{-1}X\big)^{2k+1} = \sum_{k=0}^{\tilde a_l}\mathcal{C}^{\mathrm{o}}_{k,l}(r,s)\big(h^{-1}X\big)^{2k}.$$

Thus multiplying two symbols $\lambda_{-l}$ and $\lambda_{1-j+l}$ and next dividing by $2\lambda_1$, we obtain:

$$-\frac{\lambda_{-l}\lambda_{1-j+l}}{2\lambda_1} = (\mathrm{i})^{j+3}\lambda_1^{-j}(h^{-1})^{j+1}\big(P^{\mathrm{e}}_{-l}P^{\mathrm{e}}_{1-j+l} + P^{\mathrm{e}}_{-l}P^{\mathrm{o}}_{1-j+l} + P^{\mathrm{o}}_{-l}P^{\mathrm{e}}_{1-j+l} + P^{\mathrm{o}}_{-l}P^{\mathrm{o}}_{1-j+l}\big)$$
$$= (\mathrm{i})^{j+3}\lambda_1^{-j}\big(h^{-1}\big)^{j+1}\big(A^{\mathrm{e}}_1 + B^{\mathrm{o}}_1 + B^{\mathrm{o}}_2 + A^{\mathrm{e}}_2\big).$$

Let us introduce the following set:

$$F_{a,d} = \big\{(\alpha,\beta) \in \mathbb{N}^2 \mid \alpha+\beta = d,\ 0 \leqslant \alpha \leqslant a_l,\ 0 \leqslant \beta \leqslant a_{j-1-l}\big\}.$$

Thanks to the formula of product of two polynomials, quantity $A^{\mathrm{e}}_1$ can be expressed as:

$$P^{\mathrm{e}}_{-l}P^{\mathrm{e}}_{1-j+l} = \sum_{k=0}^{a_l}\mathcal{C}^{\mathrm{e}}_{k,l}\big(h^{-1}X\big)^{2k}\sum_{m=0}^{a_{j-1-l}}\mathcal{C}^{\mathrm{e}}_{m,1-j+l}(h^{-1}X)^{2m}$$

$$= \sum_{d=0}^{a_l+a_{-1+j-l}} \left( \sum_{(\alpha,\beta)\in F_{a,d}} \mathcal{C}^{\mathrm{e}}_{\alpha,l}\mathcal{C}^{\mathrm{e}}_{\beta,-1+j-l} \right) \left(h^{-1}X\right)^{2d},$$

where we set

$$\mathcal{C}^{\mathrm{e}}_{\alpha,l} = \sum_{\rho=b_{l,\alpha}}^{c_l} A^{\mathrm{e}}_{\alpha,\rho}(h^{-1}r)^{\rho} \quad \text{and} \quad \mathcal{C}^{\mathrm{e}}_{\beta,-1+j-l} = \sum_{\rho=b_{j-1-l,\beta}}^{c_{j-1-l}} A^{\mathrm{e}}_{\beta,\rho}(s)(h^{-1}r)^{\rho}.$$

By multiplication, we deduce that:

$$P^{\mathrm{e}}_{-l}P^{\mathrm{e}}_{1-j+l} = \sum_{d=0}^{a_l+a_{j-1-l}} \left( \sum_{(\alpha,\beta)\in F_{a,d}} \left( \sum_{\delta=b_{l,\alpha}+b_{j-1-l,\beta}}^{c_l+c_{j-1-l}} \right.\right.$$
$$\left.\left. \times \left( \sum_{(\rho_1,\rho_2)\in F_{(b,c),\delta}} \left(A^{\mathrm{e}}_{\alpha,\rho_1}(s)A^{\mathrm{e}}_{\beta,\rho_2}(s)\right)\left(h^{-1}r\right)^{\delta} \right)\right)\right)\left(h^{-1}X\right)^{2d},$$

where $F_{(b,c),\delta} = \{(\rho_1,\rho_2)\in\mathbb{N}^2 \mid \rho_1+\rho_2=\delta,\ b_{l,\alpha}\leqslant\rho_1\leqslant c_l,\ b_{j-1-l,\beta}\leqslant\rho_2\leqslant c_{j-1-l}\}$. Then, we have the equalities:

$$A^{\mathrm{e}}_{\alpha,\rho_1}(s)A^{\mathrm{e}}_{\beta,\rho_2}(s) = \left\langle C_{\alpha,\rho_1}, D^{(l+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{\alpha,\rho_1}}\right\rangle_{(l+1)^{\#}}\left\langle C_{\beta,\rho_2}, D^{(j-l)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{\beta,\rho_2}}\right\rangle_{(j-l)^{\#}}$$

with $\delta_{\alpha,\rho_1}\in\tilde{\mathbb{E}}_{l+1}$ and $\delta_{\beta,\rho_2}\in\tilde{\mathbb{E}}_{j-l}$. A detailed study of this product (quite similar to the one developed during the proof of Lemma 15) shows that, even if some vanishing rational coefficients have to be added to give a sense to the scalar product in $\mathbb{R}^{(j+1)^{\#}}$ and the condition $\delta_p^{(j+1)}(d,\delta)\equiv 0$, $\forall p\in\{1,\dots,(j+1)^{\#}\}$, must be imposed to check that the maximal order of the derivatives is $(j+1)$, this last expression can be rewritten as:

$$A^{\mathrm{e}}_{\alpha,\rho_1}A^{\mathrm{e}}_{\beta,\rho_2} = \left\langle C_{\alpha,\beta,\delta}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{d,\delta}}\right\rangle_{(j+1)^{\#}}.$$

It follows from the properties on the exponents $\delta_{\alpha,\rho_1}$ and $\delta_{\beta,\rho_2}$ that we have $\delta_{d,\delta}\in\tilde{\mathbb{E}}_{j+1}$.

Let us now describe the set of elements $\delta = b_{l,\alpha}+b_{j-1-l,\beta}$ where $(\alpha,\beta)\in F_{a,d}$. By definition, $\delta$ is given by:

$$\delta = 2(\alpha-1-l)H\big(\alpha-(l+2)\big) + 2(\beta-1-(j-1-l)H\big(\beta-\big((j-1-l)+2\big)\big).$$

To suitably initialize the sum on $\delta$, we prove by a thorough study that: $\delta\geqslant b_{j,d}$.

Let us examine now the behavior of the quantities: $a_l+a_{j-1-l}$ and $c_l+c_{j-1-l}$. To achieve this, we need the two following lemmas:

LEMMA 8. – *According to the parity of $p$, the sequences of indices $\{a_p\}_{p\geqslant 0}$, $\{\tilde{a}_p\}_{p\geqslant 0}$, $\{c_p\}_{p\geqslant 0}$ and $\{\tilde{c}_p\}_{p\geqslant 0}$ can also be expressed as*:

| | |
|---|---|
| $p \geqslant 0$<br>$a_{2p} = 3p + 1$<br>$a_{2p+1} = 3p + 3$ | $c_0 = 0$<br>$p \geqslant 1$<br>$c_{2p} = 2p$<br>$c_{2p+1} = 2p + 2$ |
| $p \geqslant 0$<br>$\tilde{a}_{2p} = 3p + 1$<br>$\tilde{a}_{2p+1} = 3p + 2$ | $p \geqslant 0$<br>$\tilde{c}_{2p} = 2p + 1$<br>$\tilde{c}_{2p+1} = 2p + 1$ |

LEMMA 9. – *Set* $\dot{a} \equiv a_{p+q+1}$, $\dot{\tilde{a}} \equiv \tilde{a}_{p+q+1}$, $\dot{c} \equiv c_{p+q+1}$ *and* $\dot{\tilde{c}} \equiv \tilde{c}_{p+q+1}$. *Let* $\tau$ *and* $\sigma$ *be two non-negative integers. We then have the following rules of summation*:

| $a_q + a_p$ | $p = 2\tau$ | $p = 2\tau + 1$ |
|---|---|---|
| $q = 2\sigma$ | $\dot{a} - 1$<br>$\dot{\tilde{a}}$ | $\dot{a}$<br>$\dot{\tilde{a}}$ |
| $q = 2\sigma + 1$ | $\dot{a}$<br>$\dot{\tilde{a}}$ | $\dot{a}$<br>$\dot{\tilde{a}} + 1$ |

| $\widetilde{a}_q + \widetilde{a}_p$ | $p = 2\tau$ | $p = 2\tau + 1$ |
|---|---|---|
| $q = 2\sigma$ | $\dot{a} - 1$<br>$\dot{\tilde{a}}$ | $\dot{a} - 1$<br>$\dot{\tilde{a}} - 1$ |
| $q = 2\sigma + 1$ | $\dot{a} - 1$<br>$\dot{\tilde{a}} - 1$ | $\dot{a} - 2$<br>$\dot{\tilde{a}} - 1$ |

| $a_q + \widetilde{a}_p$ | $p = 2\tau$ | $p = 2\tau + 1$ |
|---|---|---|
| $q = 2\sigma$ | $\dot{a} - 1$<br>$\dot{\tilde{a}}$ | $\dot{a} - 1$<br>$\dot{\tilde{a}} - 1$ |
| $q = 2\sigma + 1$ | $\dot{a}$<br>$\dot{\tilde{a}}$ | $\dot{a} - 1$<br>$\dot{\tilde{a}}$ |

| $c_q + c_p$ | $p = 2\tau$ | $p = 2\tau + 1$ |
|---|---|---|
| $q = 2\sigma$ | $\dot{c} - 2$<br>$\dot{\tilde{c}} - 1$ | $\dot{c}$<br>$\dot{\tilde{c}} - 1$ |
| $q = 2\sigma + 1$ | $\dot{c}$<br>$\dot{\tilde{c}} - 1$ | $\dot{c}$<br>$\dot{\tilde{c}} + 1$ |

| $\widetilde{c}_q + \widetilde{c}_p$ | $p = 2\tau$ | $p = 2\tau + 1$ |
|---|---|---|
| $q = 2\sigma$ | $\dot{c}$<br>$\dot{\tilde{c}} + 1$ | $\dot{c}$<br>$\dot{\tilde{c}} - 1$ |
| $q = 2\sigma + 1$ | $\dot{c}$<br>$\dot{\tilde{c}} - 1$ | $\dot{c} - 2$<br>$\dot{\tilde{c}} - 1$ |

| $\widetilde{c}_q + c_p$ | $p = 2\tau$ | $p = 2\tau + 1$ |
|---|---|---|
| $q = 2\sigma$ | $\dot{c} - 1$<br>$\dot{\tilde{c}}$ | $\dot{c} + 1$<br>$\dot{\tilde{c}}$ |
| $q = 2\sigma + 1$ | $\dot{c} - 1$<br>$\dot{\tilde{c}} - 2$ | $\dot{c} - 1$<br>$\dot{\tilde{c}}$ |

From the previous lemma, if $l$ and $(j - 1 - l)$ are even (so $j$ is odd), then we deduce that: $c_l + c_{j-1-l} = c_j - 2$, and otherwise $c_l + c_{j-1-l} = c_j$. Consequently, if we consider this last case which is the larger upper bound, we get:

$$P^{\mathrm{e}}_{-l}P^{\mathrm{e}}_{1-j+l}(X)$$
$$= \sum_{d=0}^{a_l+a_{j-1-l}} \left( \sum_{(\alpha,\beta)\in F_{a,d}} \left( \sum_{\delta=b_{j,d}}^{c_j} \langle C_{\alpha,\beta,\delta}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{d,\delta}}\rangle_{(j+1)_\#} \left(h^{-1}r\right)^{\delta} \right) \left(h^{-1}X\right)^{2d} \right).$$

This expression can be reduced to:

$$P^{\mathrm{e}}_{-l}P^{\mathrm{e}}_{1-j+l}(X) = \sum_{d=0}^{a_l+a_{j-1-l}} \left( \sum_{\delta=b_{j,d}}^{c_j} \langle \tilde{C}_{d,\delta}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{d,\delta}}\rangle_{(j+1)_\#} \left(h^{-1}r\right)^{\delta} \left(h^{-1}X\right)^{2d} \right).$$

If we assume that $l$ is even and $j$ odd, then $a_l + a_{j-1-l}$ is equal to $= a_j - 1$ and $a_j$ otherwise. So, always in the larger case, we can conclude that the following writting can be adopted

$$P^{\mathrm{e}}_{-l}P^{\mathrm{e}}_{1-j+l}(X) = \sum_{d=0}^{a_j} \left( \sum_{\delta=b_{j,d}}^{c_j} \langle \tilde{C}_{d,\delta}, D^{(j+1)}(\kappa)^{\otimes\delta^{\mathrm{e}}_{d,\delta}}\rangle_{(j+1)_\#} \left(h^{-1}r\right)^{\delta} \left(h^{-1}X\right)^{2d} \right),$$

and is consistent with the desired form. Constants $\tilde{C}_{d,\delta}$ are some elements of $\mathbb{Q}^{(j+1)^\#}$ (which can vanish) and exponents $\delta^{\mathrm{e}}_{d,\delta}$ own to $\tilde{\mathbb{E}}_{j+1}$.

The analysis of the last three remaining terms, i.e. $A^{\mathrm{e}}_2$, $B^{\mathrm{o}}_1$ and $B^{\mathrm{o}}_2$, is almost the same as above. The main difference is that the exponents arising in the odd quantities $B^{\mathrm{o}}_1$ and $B^{\mathrm{o}}_2$ are in $\mathbb{E}^*_{j+1}$. $\square$

### 4.6. Product term with derivatives in expression (20)

We now study the quantity:

$$\frac{1}{2\lambda_1}\left\{ \sum_{\alpha=1}^{j+1} \frac{(-\mathrm{i})^{\alpha}}{\alpha!} \sum_{l=-1}^{j-\alpha} \partial^{\alpha}_{\xi}\lambda_{-l}\,\partial^{\alpha}_{s}\lambda_{1-j+l+\alpha} \right\}.$$

Since by assumption each symbol $\{\lambda_{-l}\}_{l=-1}^{j-1} \in \mathbb{S}^{-l}_M$ can be written under the form (12)–(13), this is quite natural to begin by studying the different terms:

- $\partial^p_\xi(\lambda_1^{-l})$ and $\partial^p_s(\lambda_1^{-l})$,
- and next $\partial^p_\xi(X^\alpha\lambda_1^{-\beta})$ and $\partial^p_s(X^\alpha\lambda_1^{-\beta})$.

#### 4.6.1. High-order derivation of powers of the principal symbol

In this section, we are interested in the computation of the terms $\partial^p_\xi(\lambda_1^{-l})$ and $\partial^p_s(\lambda_1^{-l})$, where $l \geqslant -1$. To this end, it is useful to define the set of multiindices:

$$E^*_{p,\gamma} = \left\{\beta \in \mathbb{N}^{p+1} \mid \alpha = (0,1,\ldots,p) \text{ and } \alpha\cdot\beta = p, |\beta| = \gamma, \beta_0 = 0\right\}.$$

Under these notations, we can announce the following result:

PROPOSITION 10. – *Let $p \in \mathbb{N}$ and $q = [p/2]$ be the low integer part of $p/2$. Then, $\partial^p_\xi(\lambda_1^{-l})$ satisfies*

$$\partial^p_\xi\left(\lambda_1^{-l}\right) = \lambda_1^{-l}(h\lambda_1)^{-p} \sum_{\tau=0}^{q} c_\tau \left(h^{-1}X\right)^{2\tau+p-2q}, \tag{21}$$

*for some constants $c_\tau$ of $\mathbb{Q}^+$.*

*Proof. –* One more time, the proof follows from some recursive arguments on the order of derivation $p$. By a straightforward calculation, we begin to remark that $\partial_\xi(\lambda_1^{-l}) = lh^{-2}\lambda_1^{-(l+1)}X$. So, relation (21) holds for $p = 1$.

Now, we assume that the formula is fulfilled at a fixed order of derivation $p$

$$\partial_\xi^p\big(\lambda_1^{-l}\big) = \lambda_1^{-(l+p)}h^{-p}\sum_{\tau=0}^{[p/2]} c_\tau\big(h^{-1}X\big)^{2\tau+p-2[p/2]}.$$

We then can rewrite it equivalently as:

$$\partial_\xi^p\big(\lambda_1^{-l}\big) = h^{-p-(p-2[p/2])}\sum_{\tau=0}^{[p/2]} c_\tau h^{-2\tau}\xi^{2\tau+(p-2[p/2])}\lambda_1^{-(l+p+2\tau+(p-2[p/2]))}.$$

Deriving this expression with respect to $\xi$, we obtain:

$$\begin{aligned}\partial_\xi^{p+1}\big(\lambda_1^{-l}\big) = h^{-p-(p-2[p/2])}\Bigg(&\sum_{\tau=1+[p/2]-[(p+1)/2]}^{[p/2]} c_\tau h^{-2\tau}X^{2\tau-1+(p-2[p/2])}\lambda_1^{-(l+p+1)}\\ &+\sum_{\tau=0}^{[p/2]} c_\tau h^{-2\tau}X^{2\tau+(p-2[p/2])}h^{-2}X\lambda_1^{-(l+p+1)}\Bigg),\end{aligned}$$

which can also be rewritten as:

$$\begin{aligned}\partial_\xi^{p+1}\big(\lambda_1^{-l}\big) &= \lambda_1^{-(l+p+1)}h^{-(p+1)}\Bigg(\sum_{\tau=1+[p/2]-[(p+1)/2]}^{[p/2]} c_\tau^1\big(h^{-1}X\big)^{2\tau-1+(p-2[p/2])}\\ &\qquad+\sum_{\tau=0}^{[p/2]} c_\tau^2\big(h^{-1}X\big)^{2\tau+1+(p-2[p/2])}\Bigg)\\ &= \lambda_1^{-(l+p+1)}h^{-(p+1)}(A+B),\end{aligned}$$

where $A$ and $B$ stand for each sum taken in the previous expression, $c_\tau^1$ and $c_\tau^2$ being defined in $\mathbb{Q}^+$. Then, $A$ is equal to

$$A = \sum_{\tau=1+[p/2]-[(p+1)/2]}^{[p/2]} c_\tau^1\big(h^{-1}X\big)^{2(\tau-1+[(p+1)/2]-[p/2])+(p+1-2[(p+1)/2])},$$

and after a change of the summation index

$$A = \sum_{\tau=0}^{[(p+1)/2]-1} c_\tau^1\big(h^{-1}X\big)^{2\tau+(p+1-2[(p+1)/2])}.$$

From similar arguments, $B$ has the following expression:

$$B = \sum_{\tau=[(p+1)/2]-[p/2]}^{[(p+1)/2]} c_\tau^2\big(h^{-1}X\big)^{2\tau+(p+1-2[(p+1)/2])}.$$

This finally allows us to conclude that there exist some constants $c_\tau \in \mathbb{Q}^+$, $0 \leqslant \tau \leqslant [(p+1)/2]$, such that at the order $(p+1)$ of derivation we get:

$$\partial_\xi^{p+1}(\lambda_1^{-l}) = \lambda_1^{-(l+p+1)} h^{-(p+1)} \sum_{\tau=0}^{[(p+1)/2]} c_\tau (h^{-1}X)^{2\tau+(p+1-2[(p+1)/2])}. \qquad \square$$

We now derive a similar result for $\partial_s^p(\lambda_1^{-l})$. More precisely, we have the:

PROPOSITION 11. – *Symbol $\partial_s^p(\lambda_1^{-l})$ is given by the relation*

$$\partial_s^p(\lambda_1^{-l}) = -\lambda_1^{-l} \sum_{\tau=1}^{p} \left( \sum_{\omega=3\tau}^{2\tau+p} c_{\omega,\tau} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta_{\omega,\tau}^k} h^{-\omega} (-r)^{\omega-2\tau-1} \right) r X^{2\tau}, \tag{22}$$

*where $p \in \mathbb{N}^*$, $l \leqslant -1$ and $\delta_{\omega,\tau} = (\delta_{\omega,\tau}^k)_{0\leqslant k \leqslant p} \in E_{p,\omega-2\tau-1}^*$. At last, constants $c_{\omega,\tau}$ are some elements of $\mathbb{Q}^+$.*

*Proof.* – The result is proved recursively on the order $p$ of derivation. To initialize the proof, let us remark that we directly have $\partial_s(\lambda_1^{-l}) = -lrh^{-3}\kappa' X^2 \lambda_1^{-l}$.

Let us make the assumption that equation (22) is fulfilled at the order $p$ of derivation. Deriving it according to the curvilinear abscissa $s$, we obtain:

$$\begin{aligned}
\partial_s^{p+1}(\lambda_1^{-l}) = {} & -\partial_s(\lambda_1^{-l}) \sum_{\tau=1}^{p} \left( \sum_{\omega=3\tau}^{2\tau+p} c_{\omega,\tau} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta_{\omega,\tau}^k} h^{-\omega} (-r)^{\omega-2\tau-1} \right) r X^{2\tau} \\
& - \lambda_1^{-l} \sum_{\tau=1}^{p} \partial_s \left( \sum_{\omega=3\tau}^{2\tau+p} c_{\omega,\tau} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta_{\omega,\tau}^k} h^{-\omega} (-r)^{\omega-2\tau-1} \right) r X^{2\tau} \\
& - \lambda_1^{-l} \sum_{\tau=1}^{p} \left( \sum_{\omega=3\tau}^{2\tau+p} c_{\omega,\tau} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta_{\omega,\tau}^k} h^{-\omega} (-r)^{\omega-2\tau-1} \right) r \partial_s(X^{2\tau}), \\
= {} & A + B + C,
\end{aligned}$$

where $A$, $B$ and $C$ are each of the three previous sums. Let us examine each term. We have

$$A = -\lambda_1^{-l} \sum_{\tau=1}^{p} \left( \sum_{\omega=3\tau}^{2\tau+p} \kappa' c_{\omega,\tau}(s) h^{-\omega-3} (-r)^{\omega-2\tau} \right) r X^{2(\tau+1)},$$

where we assume that $c_{\omega,\tau}(s) = c_{\omega,\tau} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta_{\omega,\tau}^k}$. By setting $\tau+1 = t$ and $w = \omega+3$, we conclude that:

$$A = -\lambda_1^{-l} \sum_{t=2}^{p+1} \left( \sum_{w=3t}^{2t+p+1} \kappa' c_{w,t}(s) h^{-w} (-r)^{w-2t-1} \right) r X^{2t}.$$

Now, let us remark that, for $c_{\omega,\tau}(s)$, we get $\delta_{\omega,\tau} \in E_{p,\omega-2\tau-1}^*$; for $c_{w,t}(s)$, we then show that $\delta_{w,t} \in E_{p,w-2t-2}^*$. As a consequence, $\kappa' c_{w,t}(s)$ can be written $\kappa' c_{w,t}(s) = \tilde{c}_{\omega,\tau} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta_{\omega,\tau}^k}$, with $\delta_{\omega,\tau} \in E_{p+1,\omega-2\tau-1}^*$. So, $A$ contributes to the higher order derivation term. It is easy to see that $C$ gives exactly the same kind of contribution.

Let us study $B$. By an expansion, we deduce that:

$$B = -\lambda_1^{-l} \sum_{\tau=1}^{p} \left( \sum_{\omega=3\tau}^{2\tau+p} \left[ \partial_s c_{\omega,\tau}(s) h^{-\omega} + c_{\omega,\tau}(s)(-r)\kappa' h^{-\omega-1} \right] (-r)^{\omega-2\tau-1} \right) r X^{2\tau} = B_1 + B_2,$$

where $B_1$ and $B_2$ are each of the terms in the brackets in the above sum. We get for $B_1$:

$$\partial_s c_{\omega,\tau}(s) = c_{\omega,\tau} \partial_s \left[ \left(\partial_s^1\right)^{\delta^1_{\omega,\tau}} \cdots \left(\partial_s^q\right)^{\delta^q_{\omega,\tau}} \cdots \left(\partial_s^p\right)^{\delta^p_{\omega,\tau}} \right] = \sum_{\substack{q=1 \\ \delta^q_{\omega,\tau} \geqslant 1}}^{p} c_{\omega,\tau,q} \left(\partial_s^q\right)^{\delta^q_{\omega,\tau}-1} \partial_s^{q+1} \prod_{\substack{k=1 \\ k \neq q}}^{p} \left(\partial_s^k\right)^{\delta^k_{\omega,\tau}},$$

with $c_{\omega,\tau,q} \in \mathbb{Q}^+$. Moreover, we also have: $c_{w,t} \prod_{k=0}^{p} (\partial_s^k \kappa)^{\delta^k_{w,t}}$, with $\delta_{w,t} \in E^*_{p+1,w-t-1}$. This last term increases the degree of derivation. Furthermore, it is easy to check that $B_2$ gives a similar contribution as $A$ and $C$. The calculation of the whole sum finally ends the proof. □

#### 4.6.2. High-order derivation of the terms $X^\alpha \lambda_1^{-\beta}$

Let us now focus our attention on the computation of high-order derivatives of $X^\alpha \lambda_1^{-\beta}$. Let us first notice the following direct consequence of Proposition 11.

COROLLARY 1. – *Let $(\alpha, \beta) \in \mathbb{N}^2$. We then have the relation*

$$\partial_s^p \left(\xi^\alpha \lambda_1^{-\beta}\right) = -\xi^\alpha \lambda_1^{-\beta} \sum_{\tau=1}^{p} \left( \sum_{\omega=3\tau}^{2\tau+p} c_{\omega,\tau} \prod_{k=0}^{p} \left(\partial_s^k \kappa\right)^{\delta^k_{\omega,\tau}} h^{-\omega} (-r)^{\omega-2\tau-1} \right) r X^{2\tau},$$

*where $\delta_{\omega,\tau} \in E^*_{p,\omega-2\tau-1}$ and $c_{\omega,\tau} \in \mathbb{Q}^+$.*

The following proposition gives a description of $\partial_\xi^p (\xi^\alpha \lambda_1^{-\beta})$.

PROPOSITION 12. – *Let $(\alpha, \beta) \in \mathbb{N}^2$. The following relations hold*:

$$\partial_\xi^p \left(\xi^\alpha \lambda_1^{-\beta}\right) = \begin{cases} h^{\alpha-p} \lambda_1^{-(\beta+p-\alpha)} \displaystyle\sum_{\tau=0}^{[(p+\alpha)/2]} c_\tau \left(h^{-1} X\right)^{2\tau + (\alpha+p-2[\frac{\alpha+p}{2}])}, & \text{if } \alpha \leqslant p, \\ \lambda_1^{-\beta} \xi^{\alpha-p} \displaystyle\sum_{\tau=0}^{p} c_\tau \left(h^{-1} X\right)^{2\tau}, & \text{if } \alpha > p, \end{cases}$$

*where $p \in \mathbb{N}$ and $c_\tau \in \mathbb{Q}^+$.*

*Proof.* – An application of the Leibniz's derivation rule yields the decomposition

$$\partial_\xi^p \left(\xi^\alpha \lambda_1^{-\beta}\right) = \sum_{k=0}^{p} C_p^k \partial_\xi^k \xi^\alpha \partial_\xi^{p-k} \left(\lambda_1^{-\beta}\right), \tag{23}$$

for any $p \in \mathbb{N}$.

*First case*. Let us assume that $\alpha \leqslant p$. Two possible cases must be distinguished:

$$\partial_\xi^k \xi^\alpha = \begin{cases} 0, & \text{if } \alpha < k, \\ \dfrac{\alpha!}{(\alpha-k)!} \xi^{\alpha-k}, & \text{otherwise.} \end{cases} \tag{24}$$

Using equation (24), relation (23) can be simpified as

$$\partial_\xi^p\big(\xi^\alpha\lambda_1^{-\beta}\big)=\sum_{k=0}^{\alpha}C_p^k\partial_\xi^k\xi^\alpha\partial_\xi^{p-k}\big(\lambda_1^{-\beta}\big),$$

where $C_p^k$ are the binomial coefficients. Proposition 10 asserts that by putting together terms in $h^{-1}X$

$$\partial_\xi^p\big(\xi^\alpha\lambda_1^{-\beta}\big)=h^{\alpha-p}\lambda_1^{-(\beta+p-\alpha)}\sum_{k=0}^{\alpha}C_p^k\frac{\alpha!}{(\alpha-k)!}\sum_{\tau=0}^{[(p-k)/2]}c_\tau\big(h^{-1}X\big)^{\alpha+2\tau+p-2k-2[(p-k)/2]}.$$

Let us now focus on the variations of the powers of $h^{-1}X$. We have:

$$\alpha+2\tau+p-2k-2\left[\frac{p-k}{2}\right]=2\left(\tau-k+\left[\frac{p+\alpha}{2}\right]-\left[\frac{p-k}{2}\right]\right)+\left((\alpha+p)-2\left[\frac{p+\alpha}{2}\right]\right).$$

The term $(\alpha+p)-2[(p+\alpha)/2]$ only gives an information about the parity of $(\alpha+p)$. We can now easily see that $\tau-k+[(p+\alpha)/2]-[(p-k)/2]$ varies in $[0,[(p+\alpha)/2]]$. These bounds correspond to $k=\alpha,\ \tau=0$ and $k=0,\ \tau=[(p-\alpha)/2]$. We can finally write $\partial_\xi^p(\xi^\alpha\lambda_1^{-\beta})$ as

$$\partial_\xi^p\big(\xi^\alpha\lambda_1^{-\beta}\big)=h^{\alpha-p}\lambda_1^{-(\beta+p-\alpha)}\sum_{\tau=0}^{[(p+\alpha)/2]}c_\tau\big(h^{-1}X\big)^{2\tau+(\alpha+p-2[(\alpha+p)/2])}$$

with $c_\tau\in\mathbb{Q}^+$.

*Second case.* Let us suppose now that $\alpha>p$. Leibniz's formula gives:

$$\partial_\xi^p\big(\xi^\alpha\lambda_1^{-\beta}\big)=\sum_{k=0}^{p}C_p^k\partial_\xi^k\xi^\alpha\partial_\xi^{p-k}\big(\lambda_1^{-\beta}\big).$$

From some similar arguments as above, we prove that:

$$\partial_\xi^p\big(\xi^\alpha\lambda_1^{-\beta}\big)=\xi^{\alpha-p}\lambda_1^{-\beta}\sum_{k=0}^{p}c_k\xi^{p-k}\lambda_1^{-\beta}h^{k-p}\lambda_1^{k-p}\sum_{\tau=0}^{[(p-k)/2]}c_\tau\big(h^{-1}X\big)^{2\tau+(p-k-2[(p-k)/2])},$$

where $c_\tau$ and $c_k$ are some constants of $\mathbb{Q}^+$. Finally, ordering the different quantities, one can reformulate the latter expression as

$$\partial_\xi^p\big(\xi^\alpha\lambda_1^{-\beta}\big)=\xi^{\alpha-p}\lambda_1^{-\beta}\sum_{k=0}^{p}c_k\sum_{\tau=0}^{[(p-k)/2]}c_\tau\big(h^{-1}X\big)^{2(\tau+p-k-[(p-k)/2])}.$$

An easy calculation shows that $\tau+p-k-[(p-k)/2]$ varies in $[0,p]$. This completes the proof. □

Combining Corollary 1 and Proposition 12 gives the following result:

COROLLARY 2. – *For any pair of indices* $(\alpha,\beta)\in\mathbb{N}^2$, *we have the relation*:

$$\partial_s^p\big(X^\alpha\lambda_1^{-\beta}\big)=-X^\alpha\lambda_1^{-\beta}\sum_{q=1}^{p}\left(\sum_{\omega=3q}^{2q+p}c_{q,\omega}\prod_{k=0}^{p}\big(\partial_s^k\kappa\big)^{\delta_{q,\omega}^k}h^{-\omega}(-r)^{\omega-2q-1}\right)rX^{2q},$$

*where* $\delta_{q,\omega}\in E^*_{p,\omega-2q-1}$ *and constants* $c_{q,\omega}\in\mathbb{Q}^+$. *Furthermore, we also have the equality*:

$$\partial_\xi^p\big(X^\alpha\lambda_1^{-\beta}\big)=\begin{cases}h^{\alpha-p}\lambda_1^{-(\beta+p)}\displaystyle\sum_{q=0}^{[(p+\alpha)/2]}c_q\big(h^{-1}X\big)^{2q+(\alpha+p-2[(\alpha+p)/2])}, & \textit{if } \alpha\leqslant p,\\ \lambda_1^{-(\beta+p)}X^{\alpha-p}\displaystyle\sum_{q=0}^{p}c_q\big(h^{-1}X\big)^{2q}, & \textit{if } \alpha>p.\end{cases}$$

### 4.7. High-order derivations of symbols $\boldsymbol{\lambda_{-l}}$

#### 4.7.1. Computation of $\boldsymbol{\partial_\xi^p\lambda_{-l}}$

Thanks to the above results, we can now analyze the term $\partial_\xi^p\lambda_{-l}$.

PROPOSITION 13. – *Symbol* $\partial_\xi^p\lambda_{-l}$, *for every* $p\geqslant 1$ *and* $l\geqslant 0$, *can be written under the following form*:

$$\partial_\xi^p\lambda_{-l}=(\mathrm{i})^{l+3}\big(h^{-1}\big)^{l+p+1}\lambda_1^{-(l+p)}\left\{\sum_{k=p-2[p/2]}^{a_l+p/2}\ \sum_{\rho=b_{l,k-(p-2[p/2])}}^{c_l}A'_{k,\rho}(s)\big(h^{-1}r\big)^\rho\big(h^{-1}X\big)^{2k}\right.$$
$$\left.+\sum_{k=p+1-2[(p+1)/2]}^{\widetilde{a}_l+(p+1)/2}\ \sum_{\rho=\widetilde{b}_{l,k-(p+1-2[(p+1)/2])}}^{\widetilde{c}_j}B'_{k,\rho}(s)\big(h^{-1}r\big)^\rho\big(h^{-1}X\big)^{2k+1}\right\},$$

*where* $A'_{k,\rho}$ *and* $B'_{k,\rho}$ *are defined as in Theorem* 5 *for some constants* $C^{\mathrm{e,o}}_{k,\rho}\in\mathbb{Q}^{(l+1)^\#}$ *and some exponents* $\delta^{\mathrm{e}}_{k,\rho}\in\widetilde{\mathbb{E}}_{l+1}$ *and* $\delta^{\mathrm{o}}_{k,\rho}\in\mathbb{E}^*_{l+1}$.

*Proof.* – Let us denote by $\lambda^{\mathrm{e}}_{-l}$ the even part of the expression of $\lambda_{-l}$ given by equation (16)

$$\lambda^{\mathrm{e}}_{-l}=(\mathrm{i})^{l+3}\lambda_1^{-l}\big(h^{-1}\big)^{l+1}\sum_{k=0}^{a_l}\sum_{\rho=b_{l,k}}^{c_l}\big(A_{k,\rho}\big(h^{-1}r\big)^\rho\big)\big(h^{-1}X\big)^{2k}.$$

Applying the differential operator $\partial_\xi^p$ and Corollary 2, we deduce the equality:

$$\partial_\xi^p\lambda^{\mathrm{e}}_{-l}=(\mathrm{i})^{l+3}\big(h^{-1}\big)^{l+p+1}\lambda_1^{-(l+p)}\left\{\sum_{\substack{k=0\\2k\leqslant p}}^{a_l}\sum_{\rho=b_{l,k}}^{c_l}\big(A_{k,\rho}\big(h^{-1}r\big)^\rho\big)\sum_{q=0}^{k+[p/2]}c_q\big(h^{-1}X\big)^{2q+(p-2[p/2])}\right.$$
$$\left.+\sum_{\substack{k=0\\2k>p}}^{a_l}\sum_{\rho=b_{l,k}}^{c_l}\big(A_{k,\rho}\big(h^{-1}r\big)^\rho\big)\sum_{q=0}^{p}c_q\big(h^{-1}X\big)^{2q+2k-p}\right\}.$$

Set $\widetilde{q}=q+k-p+[p/2]$. Since we have: $k-(p-[p/2])\geqslant 0$, if $2k>p$, this last relation can also be expressed as:

$$
\begin{aligned}
\partial_\xi^p \lambda_{-l}^{\mathrm{e}} = (\mathrm{i})^{l+3}\bigl(h^{-1}\bigr)^{l+p+1}\lambda_1^{-(l+p)}\bigl(h^{-1}X\bigr)^{(p-2[p/2])} \\
\times \left\{ \sum_{k=0}^{a_l} \sum_{\rho=b_{l,k}}^{c_l} A_{k,\rho}\bigl(h^{-1}r\bigr)^{\rho} \sum_{q=0}^{k+[p/2]} c_q\bigl(h^{-1}X\bigr)^{2q} \right\},
\end{aligned}
$$

where $c_q$ are some appropriate constants of $\mathbb{Q}^+$. Making some similar manipulations on the odd part, we get the expected result. □

#### 4.7.2. Computation of $\partial_s^p \lambda_{-l}$

This subsection deals with the computation of the curvilinear derivatives of order $p$ of the $M$-quasi homogeneous symbols of order $-l$. To achieve it, we need to prove the two following preliminary lemmas.

LEMMA 14. – *The expression of the $p$-th curvilinear derivatives of $h^{-k}$ is given by*

$$
\partial_s^p\bigl(h^{-k}\bigr) = h^{-k}\sum_{q=1}^{p}\left(\sum_{\omega\leqslant p^{\#}} C_{q,\omega}\prod_{l=0}^{p}\bigl(\partial_s^l\kappa\bigr)^{\delta_{q,\omega}^l}\right)\bigl(-rh^{-1}\bigr)^q, \tag{25}
$$

*for every $p\geqslant 1$ and $k\geqslant 0$, with some exponents $\delta_{q,\omega}=(\delta_{q,\omega}^l)_{0\leqslant l\leqslant p}\in E_{p,q}^*$ and constants $C_{q,\omega}\in\mathbb{Q}^+$.*

*Proof.* – Once again, the proof is recursively obtained on the order of derivation $p$. A simple derivation yields the consistent expression: $\partial_s(h^{-k})=-kr\kappa' h^{-(k+1)}$.

Let us now assume that equation (25) is fulfilled at the order $p$. Deriving it, we obtain:

$$
\begin{aligned}
\partial_s^{p+1}\bigl(h^{-k}\bigr) &= \partial_s\bigl(h^{-k}\bigr)\sum_{q=1}^{p}\left(\sum_{\omega\leqslant p^{\#}} C_{q,\omega}\prod_{l=0}^{p}\bigl(\partial_s^l\kappa\bigr)^{\delta_{q,\omega}^l}\right)\bigl(-rh^{-1}\bigr)^q \\
&\quad + h^{-k}\sum_{q=1}^{p}\left(\sum_{\omega\leqslant p^{\#}} C_{q,\omega}\partial_s\left(\prod_{l=0}^{p}\bigl(\partial_s^l\kappa\bigr)^{\delta_{q,\omega}^l}\right)\right)\bigl(-rh^{-1}\bigr)^q \\
&\quad + h^{-k}\sum_{q=1}^{p}\left(\sum_{\omega\leqslant p^{\#}} C_{q,\omega}\prod_{l=0}^{p}\bigl(\partial_s^l\kappa\bigr)^{\delta_{q,\omega}^l}\right)\partial_s\bigl(-rh^{-1}\bigr)^q.
\end{aligned}
$$

Several remarks must be done on each of these last three terms. By multiplying the first term by $(-rh^{-1})$, the index $q$ of the sum becomes a new index $q$ varying between 2 and $p+1$. The quantity $\kappa'$ does not increase the order of the index $p$ of the product but implies that $\delta_{q,\omega}$ is an element of the set $E_{p+1,q}^*$, where $q$ is defined as above. Consider the second term. The effect of the derivative $\partial_s$ increases the index $p$ of the product to $p+1$ and shows that $\delta_{q,\omega}\in E_{p+1,q}^*$. Finally, the last term can be treated as the first one. As a consequence, the result is true for any $p\geqslant 1$ ending hence the proof. □

LEMMA 15. – *Consider $(p,q)\in\mathbb{N}^2$ two integers such that $q\geqslant p$. Let $C_1\in\mathbb{Q}^{p^{\#}}$ and $C_2\in\mathbb{Q}^{q^{\#}}$, $\delta_1\in\mathbb{E}_p$ and $\delta_2\in\mathbb{E}_q$. Then, the following equality holds*

$$
\bigl\langle C_1, D^{(p)}(\kappa)^{\otimes\delta_1}\bigr\rangle_{p^{\#}}\bigl\langle C_2, D^{(q)}(\kappa)^{\otimes\delta_2}\bigr\rangle_{q^{\#}} = \bigl\langle C_3, D^{(p+q)}(\kappa)^{\otimes\delta_3}\bigr\rangle_{(p+q)^{\#}},
$$

*for some constants $C_3\in\mathbb{Q}^{(p+q)^{\#}}$ and exponents $\delta_3\in\mathbb{E}_{p+q}$.*

*Proof.* – By definition, we can assert that:

$$\left\langle C_1, D^{(p)}(\kappa)^{\otimes\delta_1}\right\rangle_{p^\#}\left\langle C_2, D^{(q)}(\kappa)^{\otimes\delta_2}\right\rangle_{q^\#} = \left(\sum_{\alpha=1}^{p^\#} C_1^\alpha \prod_{j=0}^{p}\left(\partial_s^j\kappa\right)^{\delta_{1,\alpha}^j}\right)\left(\sum_{\beta=1}^{q^\#} C_2^\beta \prod_{l=0}^{q}\left(\partial_s^l\kappa\right)^{\delta_{2,\beta}^l}\right). \tag{26}$$

Let $\alpha$ and $\beta$ be two indices. We then have

$$C_1^\alpha C_2^\beta \prod_{j=0}^{p}\left(\partial_s^j\kappa\right)^{\delta_{1,\alpha}^j}\prod_{l=0}^{q}\left(\partial_s^l\kappa\right)^{\delta_{2,\beta}^l} = C_{12}^{\alpha,\beta}\prod_{\omega=0}^{q}\left(\partial_s^\omega\kappa\right)^{\delta_{1,2,\alpha,\beta}^{(\omega)}}, \tag{27}$$

where $C_{12}^{\alpha,\beta} = C_1^\alpha C_2^\beta$, the exponent $\delta_{1,2,\alpha,\beta}^{(\omega)}$ is such that:

$$\delta_{1,2,\alpha,\beta}^{(\omega)} = \widetilde{\delta}_{1,\alpha}^{(\omega)} + \delta_{2,\beta}^{(\omega)}, \quad 0 \leqslant \omega \leqslant q, \tag{28}$$

and where $\widetilde{\delta}_{1,\alpha}^{(\omega)}$ is the vector of $\mathbb{N}^q$ whose $p$ first components are $\delta_{1,\alpha}^{(\omega)}$ while the $(q-p)$ last ones vanish. This last relation is satisfied since we moreover assume that $q \geqslant p$. Using equations (26) and (27), it follows that:

$$\left\langle C_1, D^{(p)}(\kappa)^{\otimes\delta_1}\right\rangle_{p^\#}\left\langle C_2, D^{(q)}(\kappa)^{\otimes\delta_2}\right\rangle_{q^\#} = \sum_{\theta=1}^{p^\#+q^\#} C_3^\theta \prod_{\omega=0}^{p+q}\left(\partial_s^\omega\kappa\right)^{\delta_{3,\theta}^\omega},$$

even if certain coefficients have to be fixed to zero. Finally, since $p^\# + q^\# \leqslant (p+q)^\#$, we conclude that there exist $C_3 \in \mathbb{Q}^{(p+q)^\#}$, $\delta_3 \in \mathbb{E}_{p+q}$ such that:

$$\left\langle C_1, D^{(p)}(\kappa)^{\otimes\delta_1}\right\rangle_{p^\#}\left\langle C_2, D^{(q)}(\kappa)^{\otimes\delta_2}\right\rangle_{q^\#} = \left\langle C_3, D^{(p+q)}(\kappa)^{\otimes\delta_3}\right\rangle_{(p+q)^\#}.$$

By relation (28), we conclude that $\delta_3$ is an element of the set $\mathbb{E}_{p+q}$ since $\delta_1 \in \mathbb{E}_p$ and $\delta_2 \in \mathbb{E}_q$. □

These two lemmas allow to prove the following essential theorem.

THEOREM 16. – *Symbol $\partial_s^p\lambda_{-l}$ of order $-l$, for every $p \geqslant 1$ and $l \geqslant 0$, is given by*:

$$\begin{aligned}\partial_s^p\lambda_{-l} = {} & (\mathrm{i})^{l+3}\left(h^{-1}\right)^{l+1}\lambda_1^{-l}\\ & \times\left\{\sum_{k=0}^{a_l+p}\left[\sum_{\theta=b_{l,k}+2}^{c_l+p}\left\langle C_{k,\theta}^{\mathrm{e}}, D^{(l+1+p)}(\kappa)^{\otimes\delta_{k,\theta}^{\mathrm{e}}}\right\rangle_{(l+1+p)^\#}\left(h^{-1}r\right)^\theta\right]\left(h^{-1}X\right)^{2k}\right.\\ & \left.+\sum_{k=0}^{\tilde{a}_l+p}\left[\sum_{\theta=\tilde{b}_{l,k}+2}^{\tilde{c}_l+p}\left\langle C_{k,\theta}^{\mathrm{o}}, D^{(l+1+p)}(\kappa)^{\otimes\delta_{k,\theta}^{\mathrm{o}}}\right\rangle_{(l+1+p)^\#}\left(h^{-1}r\right)^\theta\right]\left(h^{-1}X\right)^{2k+1}\right\},\end{aligned}$$

*with some constants $C_{k,\theta}^{\mathrm{e,o}}$ of $\mathbb{Q}^{(j+1+p)^\#}$ and some exponents $\delta_{k,\theta}^{\mathrm{e}} \in \tilde{\mathbb{E}}_{l+1+p}$ and $\delta_{k,\theta}^{\mathrm{o}} \in \mathbb{E}_{l+1+p}^*$.*

*Proof.* – Let $\lambda_{-l}^{\mathrm{e}}$ be the even part of symbol $\lambda_{-l}$. Let us define $\Psi_k$ as the function given by

$$\psi_k(s) = \sum_{\rho=b_{l,k}}^{c_l} A_{k,\rho}(s)\left(h^{-1}\right)^{\rho+l+1+2k}r^\rho,$$

where we have set

$$A_{k,\rho}(s) = \langle C^{\mathrm{e}}_{k,\rho}, D^{(l+1)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \rangle_{(l+1)^{\#}},$$

for some constants $C^{\mathrm{e}}_{k,\rho} \in \mathbb{Q}^{(l+1)^{\#}}$ and exponents $\delta^{\mathrm{e}}_{k,\rho} \in \tilde{\mathbb{E}}_{l+1}$. Under these notations, we can write the odd part of symbol $\lambda^{\mathrm{e}}_{-l}$ as being equal to:

$$\lambda^{\mathrm{e}}_{-l} = (\mathrm{i})^{l+3} \sum_{k=0}^{a_l} \psi_k(s) (\lambda_1^+)^{-l} X^{2k}.$$

The application of the Leibniz's derivation rule yields

$$\partial_s^p (\lambda^{\mathrm{e}}_{-l}) = (\mathrm{i})^{l+3} \sum_{k=0}^{a_l} \left( \sum_{m=0}^{p} C_p^m \partial_s^{p-m} \psi_k(s) \partial_s^m \left( (\lambda_1^+)^{-l} X^{2k} \right) \right), \tag{29}$$

where $C_p^m$ are the binomial coefficients. The expression of symbol $\partial_s^m((\lambda_1^+)^{-l} X^{2k})$ is given by Corollary 2. Furthermore, another application of the Leibniz's formula shows that:

$$\partial_s^{p-m} \psi_k(s) = \sum_{\rho=b_{l,k}}^{c_l} r^\rho \sum_{n=0}^{p-m} C_{p-m}^n \partial_s^n A_{k,\rho} \partial_s^{p-m-n} \left[ (h^{-1})^{\rho+l+1+2k} \right]. \tag{30}$$

Lemma 14 directly implies that:

$$\begin{aligned} &\partial_s^{p-m-n} \left[ (h^{-1})^{\rho+l+1+2k} \right] \\ &\quad = h^{-(\rho+1+l+2k)} \sum_{q=1}^{p-m-n} \left( \sum_{\omega \leqslant (p-m-n)^{\#}} C_{q,\omega} \prod_{\gamma=0}^{p-m-n} \left( \partial_s^\gamma \kappa \right)^{\delta^\gamma_{q,\omega}} \right) (-r h^{-1})^q, \end{aligned} \tag{31}$$

where $\delta_{q,\omega} \in E^*_{p-m-n,q}$ and $C_{q,\omega} \in \mathbb{Q}^+$. Moreover, we can also write that

$$\partial_s^n A_{k,\rho} = \langle C^{\mathrm{e}}_{k,\rho}, \partial_s^n D^{(l+1)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \rangle_{(l+1)^{\#}}. \tag{32}$$

Using the representation formula (14), we conclude that:

$$\partial_s^n A_{k,\rho} = \langle \tilde{C}^{\mathrm{e}}_{k,\rho}, D^{(l+1+n)}(\kappa)^{\otimes \delta'^{\mathrm{e}}_{k,\rho}} \rangle_{(l+1+n)^{\#}},$$

for a matrix $\delta'^{\mathrm{e}}_{k,\rho} \in \tilde{\mathbb{E}}_{l+1+n}$ and some constants $\tilde{C}^{\mathrm{e}}_{k,\rho} \in \mathbb{Q}^{(l+1+n)^{\#}}$ determined by the application of the differential operator $\partial_s^n$. Inserting equations (31) and (32) in (30), and next expanding and ordering the different sums and products, we get:

$$\begin{aligned} &\partial_s^n A_{k,\rho} \partial_s^{p-m-n} \left[ (h^{-1})^{\rho+l+1+2k} \right] \\ &\quad = (h^{-1})^{\rho+l+1+2k} \sum_{\theta=1}^{p-m-n} \langle C_{k,\rho,\theta,m}, D^{(l+p+1-m)}(\kappa)^{\otimes \delta''_{k,\rho,\theta}} \rangle_{(l+1+p-m)^{\#}} (h^{-1} r)^\theta, \end{aligned}$$

for some coefficients $C_{k,\rho,\theta,m} \in \mathbb{Q}^{(l+1+p-m)^{\#}}$ and exponents $\delta''_{k,\rho,\theta}$ of $\tilde{\mathbb{E}}_{l+1+p-m}$. By a summation on $n$ and some linear combinations, we deduce the relation:

$$\sum_{n=0}^{p-m} C_{p-m}^n \partial_s^n A_{k,\rho} \partial_s^{p-m-n}\left[\left(h^{-1}\right)^{\rho+l+1+2k}\right]$$
$$= \left(h^{-1}\right)^{\rho+l+1+2k} \sum_{\theta=1}^{p-m} \left\langle C'_{k,\rho,\theta,m}, D^{(l+p+1-m)}(\kappa)^{\otimes\delta'''_{k,\rho,\theta}}\right\rangle_{(l+1+p-m)^\#} \left(h^{-1}r\right)^\theta,$$

with some new coefficients $C'_{k,\rho,\theta,m} \in \mathbb{Q}^{(l+1+p-m)^\#}$ and modified exponents $\delta'''_{k,\rho,\theta}$ of $\tilde{\mathbb{E}}_{l+1+p-m}$. As a consequence, we have the expression of $\partial_s^{p-m}\psi_k(s)$:

$$\partial_s^{p-m}\psi_k(s)$$
$$= \left(h^{-1}\right)^{l+1+2k} \sum_{\rho=b_{l,k}}^{c_l} \left(h^{-1}r\right)^\rho \sum_{\theta=1}^{p-m} \left\langle C'_{k,\rho,\theta,m}, D^{(l+p+1-m)}(\kappa)^{\otimes\delta'''_{k,\rho,\theta}}\right\rangle_{(l+1+p-m)^\#} \left(h^{-1}r\right)^\theta.$$

Interpreting this double sum as a linear combination of polynomial terms with respect to variable $h^{-1}r$, we can reformulate this latter expression as

$$\partial_s^{p-m}\psi_k(s) = \left(h^{-1}\right)^{1+l+2k} \sum_{\rho=b_{l,k}+1}^{c_l+p-m} \left\langle C_{\rho,m,p}, D^{(l+p+1-m)}(\kappa)^{\otimes\delta_{k,\rho}}\right\rangle_{(l+1+p-m)^\#} \left(h^{-1}r\right)^\rho,$$

for some coefficient $C_{\rho,m,p} \in \mathbb{Q}^{(l+1+p-m)^\#}$ and exponents $\delta_{k,\rho}$ of $\tilde{\mathbb{E}}_{l+1+p-m}$. Corollary 2 yields

$$\partial_s^m\left(\left(\lambda_1^+\right)^{-l} X^{2k}\right) = -X^{2k}\lambda_1^{-l} \sum_{q=1}^{m} \left( \sum_{\omega=3q}^{2q+m} c_{q,\omega} \prod_{k=0}^{m} \left(\partial_s^k\kappa\right)^{\delta_{q,\omega}^k} h^{-\omega}(-r)^{\omega-2q-1} \right) r X^{2q},$$

where $|\delta_{q,\omega}^k| = \omega - 2q - 1$. Thus using these two last relations, we obtain:

$$\partial_s^{p-m}\psi_k \partial_s^m\left(\left(\lambda_1^+\right)^{-l} X^{2k}\right)$$
$$= \left(h^{-1}X\right)^{2k}\lambda_1^{-l}\left(h^{-1}\right)^{1+l}$$
$$\times \sum_{q=1}^{m} \left( \sum_{\theta=b_{l,k}+1+q}^{c_l+p} \left\langle C_{q,\theta,m,k}, D^{(l+p+1)}(\kappa)^{\otimes\delta_{q,\theta,m,k}}\right\rangle_{(l+1+m)^\#} \left(h^{-1}r\right)^\theta \right) r X^{2q},$$

where $C_{q,\theta,m,k} \in \mathbb{Q}^{(l+1+m)^\#}$ and $\delta_{q,\theta,m,k} \in \tilde{\mathbb{E}}_{l+1+m}$. By using equation (29), some linear combinations, orderings and products of the polynomial terms with respect to $h^{-1}X$, we get the first part of the expected expression given in Theorem 16. The odd part $\lambda_{-l}^{\mathrm{o}}$ can be treated very similarly. Finally, we end the proof adding the even and odd contributions. □

#### 4.7.3. Computation of the complete sum

We are now interested in the computation of the whole sum arising in the expression (20):

$$\frac{1}{2\lambda_1}\left\{ \sum_{\alpha=1}^{j+1} \frac{(-\mathrm{i})^\alpha}{\alpha!} \sum_{l=-1}^{j-\alpha} \partial_\xi^\alpha \lambda_{-l} \partial_s^\alpha \lambda_{1-j+l+\alpha} \right\}.$$

Let us split the internal sum into three parts

$$S_\alpha = \sum_{l=-1}^{j-\alpha} \partial_\xi^\alpha \lambda_{-j} \partial_s^\alpha \lambda_{1-j+l+\alpha} = S_\alpha^{-1} + \widetilde{S_\alpha} + S_\alpha^{j-\alpha},$$

where the three partial sums are defined by the relations

$$S_\alpha^{-1} = \partial_\xi^\alpha \lambda_1 \partial_s^\alpha \lambda_{-j+\alpha}, \qquad \widetilde{S_\alpha} = \sum_{l=0}^{j-\alpha-1} \partial_\xi^\alpha \lambda_{-l} \partial_s^\alpha \lambda_{1-j+l+\alpha}, \qquad S_\alpha^{-1} = \partial_\xi^\alpha \lambda_{-j+\alpha} \partial_s^\alpha \lambda_1.$$

The reason to use such a decomposition is related to the particular form of the two symbols $\partial_\xi^\alpha \lambda_1$ and $\partial_s^\alpha \lambda_1$ involving in the calculations.

**Computation of $\widetilde{S_\alpha}$.** To simplify the proof, let us set for $0 \leqslant l \leqslant j-\alpha-1$

$$\partial_s^\alpha \lambda_{1-j+l+\alpha} = \partial_s^\alpha \lambda_{1-j+l+\alpha}^{\mathrm{e}} + \partial_s^\alpha \lambda_{1-j+l+\alpha}^{\mathrm{o}},$$

where the even and odd parts are respectively given by:

$$\partial_s^\alpha \lambda_{-L}^{\mathrm{e}} = (\mathrm{i})^{L+3}\big(h^{-1}\big)^{L+1} \lambda_1^{-L} \sum_{k=0}^{a_L+\alpha} \left( \sum_{\theta=b_{L,k}+2}^{c_L+\alpha} \big\langle C_{k,\theta}^{\mathrm{e}}, D^{(j-l)}(\kappa)^{\otimes \delta_{k,\theta}^{\mathrm{e}}} \big(h^{-1}r\big)^\theta \big\rangle_{(j-l)^\#} \right) \big(h^{-1}X\big)^{2k} \tag{33}$$

and

$$\partial_s^\alpha \lambda_{-L}^{\mathrm{o}} = (\mathrm{i})^{L+3}\big(h^{-1}\big)^{L+1} \lambda_1^{-L} \sum_{k=0}^{\tilde{a}_L+\alpha} \left( \sum_{\theta=\tilde{b}_{L,k}+2}^{\tilde{c}_L+\alpha} \big\langle C_{k,\theta}^{\mathrm{o}}, D^{(j-l)}(\kappa)^{\otimes \delta_{k,\theta}^{\mathrm{o}}} \big(h^{-1}r\big)^\theta \big\rangle_{(j-l)^\#} \right) \big(h^{-1}X\big)^{2k}. \tag{34}$$

The index $L$ is set to: $L = j-1-l-\alpha$. Proposition 25 allows us to claim that

$$\partial_\xi^\alpha \lambda_{-l} = \partial_\xi^\alpha \lambda_{-l}^{\mathrm{e}} + \partial_\xi^\alpha \lambda_{-l}^{\mathrm{o}},$$

where

$$\partial_\xi^\alpha \lambda_{-l}^{\mathrm{e}} = (\mathrm{i})^{l+3}\big(h^{-1}\big)^{l+\alpha+1} \lambda_1^{-(l+\alpha)} \left\{ \sum_{k=\alpha-2[\alpha/2]}^{a_l+\alpha/2} \sum_{\rho=b_{l,k-(\alpha-2[\alpha/2])}}^{c_l} A'_{k,\rho}(s)\big(h^{-1}r\big)^\rho \big(h^{-1}X\big)^{2k} \right\} \tag{35}$$

and

$$\begin{aligned} \partial_\xi^\alpha \lambda_{-l}^{\mathrm{o}} = {} & (\mathrm{i})^{l+3}\big(h^{-1}\big)^{l+\alpha+1} \lambda_1^{-(l+\alpha)} \\ & \times \left\{ \sum_{k=\alpha+1-2[(\alpha+1)/2]}^{\widetilde{a}_l+(\alpha+1)/2} \sum_{\rho=\widetilde{b}_{l,k-(\alpha+1-2[(\alpha+1)/2])}}^{\widetilde{c}_l} B'_{k,\rho}(s)\big(h^{-1}r\big)^\rho \big(h^{-1}X\big)^{2k+1} \right\}, \end{aligned} \tag{36}$$

with

$$A'_{k,\rho}(s) = \big\langle C_{k,\rho}^{\prime\mathrm{e}}, D^{(l+1)}(\kappa)^{\otimes \delta_{k,\rho}^{\prime\mathrm{e}}} \big\rangle_{(l+1)^\#}, \qquad B'_{k,\rho}(s) = \big\langle C_{k,\rho}^{\prime\mathrm{o}}, D^{(l+1)}(\kappa)^{\otimes \delta_{k,\rho}^{\prime\mathrm{o}}} \big\rangle_{(l+1)^\#},$$

for some coefficients $(C'^{\mathrm{e}}_{k,\rho}, C'^{\mathrm{o}}_{k,\rho}) \in \mathbb{Q}^{(l+1)^\#} \times \mathbb{Q}^{(l+1)^\#}$ and exponents $(\delta'^{\mathrm{e}}_{k,\rho}, \delta'^{\mathrm{o}}_{k,\rho}) \in \tilde{\mathbb{E}}_{l+1} \times \mathbb{E}^*_{l+1}$. This last notation must be carefully considered because symbols e and o do not necessarily designate as previously mentioned respectively an even or odd part since the parity of $A'_{k,\rho}$ and $B'_{k,\rho}$ simultaneously permute with respect to the parity of the order of derivation $\alpha$.

Let us now show that products (33)–(35), (36) and (34)–(35), (36) are both of the generic form:

$$\begin{aligned}\partial_\xi^\alpha \lambda_{-l}^{\mathrm{e,o}} \partial_s^\alpha \lambda_{-L}^{\mathrm{e,o}} &= (\mathrm{i})^{j-\alpha+1} \big(h^{-1}\big)^{j+1} \lambda_1^{1-j} \\ &\quad \times \Bigg\{ \sum_{k=0}^{a_j} \Bigg[ \sum_{\rho=b_{j,k}}^{c_j} \big\langle C^{\mathrm{e}}_{k,\rho}, D^{(j+1)}(\kappa)^{\otimes \delta^{\mathrm{e}}_{k,\rho}} \big\rangle_{(j+1)^\#} \big(h^{-1} r\big)^\rho \Bigg] \big(h^{-1} X\big)^{2k} \\ &\quad + \sum_{k=0}^{\tilde{a}_j} \Bigg[ \sum_{\rho=\tilde{b}_{j,k}}^{\tilde{c}_j} \big\langle C^{\mathrm{o}}_{k,\rho}, D^{(j+1)}(\kappa)^{\otimes \delta^{\mathrm{o}}_{k,\rho}} \big\rangle_{(j+1)^\#} \big(h^{-1} r\big)^\rho \Bigg] \big(h^{-1} X\big)^{2k+1} \Bigg\}. \end{aligned} \tag{37}$$

Let us firstly focus our attention on the maximal degree of terms $(h^{-1}X)^\theta$. Theorem 5 shows that the maximal degree $\theta_{\max}$ depends on the parity of $j$ and is equal to $2a_j$ if $j$ is odd and to $2\tilde{a}_j + 1$ otherwise. Therefore, we have to analyze the maximal degree of products $\partial_s^\alpha \lambda_{-L}^{\mathrm{type}_s} \partial_\xi^\alpha \lambda_{-l}^{\mathrm{type}_\xi}$, where $\mathrm{type}_s$ and $\mathrm{type}_\xi$ can designate the even or odd parts e and o. This gives rise to the following rules for $\theta$:

| $\partial_s^\alpha \lambda_{-L}^{\mathrm{type}_s} \partial_\xi^\alpha \lambda_{-l}^{\mathrm{type}_\xi}$ | $\mathrm{type}_\xi = \mathrm{e}$ | $\mathrm{type}_\xi = \mathrm{o}$ |
|---|---|---|
| $\mathrm{type}_s = \mathrm{e}$ | $2(a_L + a_l) + 3\alpha$ | $2(a_L + \tilde{a}_l) + 3\alpha + 1$ |
| $\mathrm{type}_s = \mathrm{o}$ | $2(\tilde{a}_L + a_l) + 3\alpha + 1$ | $2(\tilde{a}_L + \tilde{a}_l) + 3\alpha + 2$ |

In order to prove that we effectively derive a formula which falls into the scope of expression (37), we have to check that each of these exponents is lower than or equal to $2a_j$ and $2\tilde{a}_j + 1$. This is the aim of the two arrays below where we compute, according to the parity of $\alpha$, $j$ and $l$ (also fixing the parity of $L$) and using the calculation rules stated in Lemma 8, the difference between the exponents obtained in the above array and $2a_j$ if $j$ is even and $2\tilde{a}_j + 1$ otherwise. Of course, the results must be non-negative to positively conclude.

| $j$ odd (compared to $2\tilde{a}_j + 1$) | | | $(\mathrm{type}_s, \mathrm{type}_\xi)$ | | | |
|---|---|---|---|---|---|---|
| | | | (e, e) | (e, o) | (o, e) | (o, o) |
| $l$ even | $\alpha$ even | $L$ even | $-2$ | $-1$ | $-1$ | 0 |
| | $\alpha$ odd | $L$ odd | $-1$ | 0 | $-2$ | $-1$ |
| $l$ odd | $\alpha$ even | $L$ odd | 0 | $-2$ | $-2$ | $-2$ |
| | $\alpha$ odd | $L$ even | $-1$ | $-2$ | 0 | $-1$ |

| $j$ even (compared to $2a_j$) | | | $(\text{type}_s, \text{type}_\xi)$ | | | |
|---|---|---|---|---|---|---|
| | | | (e, e) | (e, o) | (o, e) | (o, o) |
| $l$ even | $\alpha$ even | $L$ odd | $-1$ | 0 | $-2$ | $-1$ |
| | $\alpha$ odd | $L$ even | $-2$ | $-1$ | $-1$ | 0 |
| $l$ odd | $\alpha$ even | $L$ even | $-2$ | $-2$ | 0 | $-1$ |
| | $\alpha$ odd | $L$ odd | 0 | $-1$ | $-1$ | $-2$ |

As seen above, there are several contributions to the higher-order general term, property which has not been still encountered until now.

A similar study can be pursued for terms in $(h^{-1}r)^\theta$. We get the following array on the maximal degrees:

| $\partial_s^\alpha \lambda_{-L}^{\text{type}_s} \partial_\xi^\alpha \lambda_{-l}^{\text{type}_\xi}$ | $\text{type}_\xi = \text{e}$ | $\text{type}_\xi = \text{o}$ |
|---|---|---|
| $\text{type}_s = \text{e}$ | $c_L + c_l + \alpha$ | $a_L + \tilde{c}_l + \alpha$ |
| $\text{type}_s = \text{o}$ | $\tilde{c}_L + c_l + \alpha$ | $\tilde{c}_L + \tilde{c}_l + \alpha$ |

which must be compared to $c_j$ or $\tilde{c}_j$ for respectively an odd or even value of $j$ since $\tilde{c}_j > c_j$ when $j$ is even (and conversely).

| $j$ odd (compared to $c_j$) | | | $(\text{type}_s, \text{type}_\xi)$ | | | |
|---|---|---|---|---|---|---|
| | | | (e, e) | (e, o) | (o, e) | (o, o) |
| $l$ even | $\alpha$ even | $L$ even | $-2$ | $-1$ | $-1$ | 0 |
| | $\alpha$ odd | $L$ odd | $-1$ | $-2$ | 0 | $-1$ |
| $l$ odd | $\alpha$ even | $L$ odd | 0 | $-1$ | $-1$ | $-2$ |
| | $\alpha$ odd | $L$ even | $-1$ | 0 | $-2$ | $-1$ |

| $j$ even (compared to $\tilde{c}_j$) | | | $(\text{type}_s, \text{type}_\xi)$ | | | |
|---|---|---|---|---|---|---|
| | | | (e, e) | (e, o) | (o, e) | (o, o) |
| $l$ even | $\alpha$ even | $L$ odd | $-1$ | $-2$ | 0 | $-1$ |
| | $\alpha$ odd | $L$ even | $-2$ | $-1$ | $-1$ | 0 |
| $l$ odd | $\alpha$ even | $L$ even | $-1$ | 0 | $-2$ | $-1$ |
| | $\alpha$ odd | $L$ odd | 0 | $-1$ | $-1$ | $-2$ |

Let us now find a lower bound for the minimal index of terms $(h^{-1}r)^\theta$. More precisely, these indices to analyze are:

$$
\begin{aligned}
&b_{L,k} + 2 + b_{l,k-(\alpha-2[\alpha/2])}, \qquad && \tilde{b}_{L,k} + 2 + b_{l,k-(\alpha-2[\alpha/2])},\\
&b_{L,k} + 2 + \tilde{b}_{l,k-(\alpha-2[\alpha/2])}, \qquad && \tilde{b}_{L,k} + 2 + \tilde{b}_{l,k-(\alpha-2[\alpha/2])}.
\end{aligned}
$$

By some almost similar arguments as were used in the proof of Proposition 2, it can be shown that $b_{j-\alpha,\rho_1+\rho_2} \leqslant b_{l,\rho_1} + b_{j-1-\alpha-l,\rho_2}$. Using the hypothesis: $1 \leqslant j-\alpha \leqslant j-1$ and next the decreasing property of $b_{\cdot,\rho_1+\rho_2}$ with respect to $j$, we get $b_{j,\rho_1+\rho_2} \leqslant b_{j-\alpha,\rho_1+\rho_2}$, $\forall \alpha \geqslant 0$. Combining these two bounds, we can conclude that:

$$\begin{aligned}\partial_\xi^\alpha \lambda_{-l} \partial_s^\alpha \lambda_{-L} = (\mathrm{i})^{j-\alpha+1}\big(h^{-1}\big)^{j+1} \lambda_1^{1-j} \\ \times \Bigg\{ \sum_{k=0}^{a_j} \Bigg[ \sum_{\rho=b_{j,k}}^{c_j} \big\langle C_{k,\rho}^{\mathrm{e}}, D^{(j+1)}(\kappa)^{\otimes \delta_{k,\rho}^{\mathrm{e}}} \big\rangle_{(j+1)^\#} \big(h^{-1}r\big)^\rho \Bigg] \big(h^{-1}X\big)^{2k} \\ + \sum_{k=0}^{\tilde a_j} \Bigg[ \sum_{\rho=\tilde b_{j,k}}^{\tilde c_j} \big\langle C_{k,\rho}^{\mathrm{o}}, D^{(j+1)}(\kappa)^{\otimes \delta_{k,\rho}^{\mathrm{o}}} \big\rangle_{(j+1)^\#} \big(h^{-1}r\big)^\rho \Bigg] \big(h^{-1}X\big)^{2k+1} \Bigg\}.\end{aligned}$$

So, by summing on $l = 0 \cdots j-\alpha-1$, we still obtain an expression of the same kind since the relation is independent on the index $l$. Finally, multiplying by $i^\alpha/\alpha!$, we prove that symbol $\widetilde{S_\alpha}/(2\lambda_1)$ has the desired form.

**Computations of $S_\alpha^{-1}$ and $S_\alpha^{j-\alpha}$.** Despite the quite specific form of $S_\alpha^{-1}$ et $S_\alpha^{j-\alpha}$, a detailed study shows that they can be involved by adaptating the proof for $\tilde{S}_\alpha$. Multiplying by $(\mathrm{i})^\alpha/\mathrm{i}!$ and next summing on $\alpha$ and finally dividing each partial sum by $2\lambda_1$ lead to the expected contribution of each term.

Consequently, it follows that the complete sum

$$\frac{1}{2\lambda_1} \sum_{\alpha=1}^{j+1} \frac{\mathrm{i}^\alpha}{\alpha} S_\alpha$$

is consistent with (16). Combining the above result and Propositions 1 and 2, we can now assert that symbol $\lambda_{-j}$ given by (20) can be characterized by the relations (16)–(17). As a by-product, this also proves the quasi-analytic characterization Theorem 5.

## 5. Fractional asymptotic artificial boundary conditions on an arbitrary fictitious boundary

This last section is devoted to the derivation of artificial boundary conditions involving time fractional derivatives for the Schrödinger equation in the "high-frequency zone" (covariable $\tau$ great compared to $\xi^2$). These conditions which result from an asymptotic analysis of the transparent operator have the property of being *local in space but non local with respect to time*. This is a straightforward consequence of the $M$-quasi homogeneous character of the principal symbol $\widetilde{\lambda_1}$ coupled with an asymptotic analysis based on a double expansion of the transparent operator both in symbols and frequency. It can be shown that according to the previous results which give a high-frequency control of the symbols that this double expansion is consistent. As a consequence, this allows us to state the definition of the order of an asymptotic condition. Finally, we give several examples of these new conditions.

### 5.1. Asymptotic artificial boundary conditions

We are interested here in both the construction and the clarification of the notion of fractional approximate artificial boundary condition with a fixed order for our model problem. Let us recall that the transparent condition (8) is given by the $M$-quasi homogeneous pseudodifferential equation:

$$Tv = (\partial_{\mathbf{n}} + \mathrm{i}\widetilde{\Lambda})v = 0, \quad \text{on } \Sigma. \tag{38}$$

As previously seen, operator $\widetilde{\Lambda}$ is an element of the class $OP\mathbb{S}^1_M$ with a total symbol $\widetilde{\lambda}$ admitting an asymptotic expansion in $M$-quasi homogeneous symbols $(\widetilde{\lambda_{-j}})_{j\geqslant -1}$ of the form

$$\widetilde{\lambda} \sim \sum_{j=-1}^{+\infty} \widetilde{\lambda_{-j}} \tag{39}$$

characterized by the quasi-analytic formula:

$$\begin{aligned}
&\widetilde{\lambda_1} = -\left(-\left(\xi^2 + \tau\right)\right)^{1/2}, \\
&\widetilde{\lambda_{-j}} = \left(\widetilde{\lambda_1}\right)^{-j} (\mathrm{i})^{j+3} \left\{ \sum_{k=0}^{j+1} A_k X^{2k} + \sum_{k=0}^{j} B_k X^{2k+1} \right\}, \quad j \geqslant 0,
\end{aligned}$$

where coefficients $A_k$ and $B_k$ are some functions of the curvatures (see Theorem 6). From a pure practical viewpoint, it is obvious that the total symbol $\widetilde{\lambda}$ can not be completely computed.

Hence we are lead to derive an approximate boundary condition truncating expansion (39). In this way, we denote by:

$$\mathcal{T}_{(m+2)} v = \left(\partial_{\mathbf{n}} + \mathrm{i}\mathrm{Op}\left(\sum_{j=-1}^{m} \widetilde{\lambda_{-j}}\right)\right) v = 0, \quad j \geqslant -1, \text{ on } \Sigma, \tag{40}$$

the approximate boundary condition obtained after having kept on the $(m+2)$ first terms of the asymptotic expansion of $\widetilde{\lambda}$. Unfortunately, this boundary condition is still defined through a *non-local* pseudodifferential operator *both in space and time*. As a consequence, the numerical implementation of such an operator is characterized by a too high computational complexity [9] to be useful in some realistic situations.

To partially find a solution to this default of the family of conditions of type (40), a second expansion is required. Let us recall that all the calculations are made in the $M$-quasi hyperbolic zone $\mathcal{H}$. So an expansion with respect to $\tau$ yields the following different controls of symbols:

$$\frac{1}{(\widetilde{\lambda_1})^j} = \mathcal{O}\left(\frac{1}{\tau^{j/2}}\right) \quad \text{and} \quad X^K = \mathcal{O}\left(\frac{1}{\tau^{K/2}}\right),$$

for $j \geqslant -1$ and $K \geqslant 0$. In particular, this implies that each symbol of order $-j$ of the asymptotic expansion of operator $\widetilde{\Lambda}$ satisfies

$$\widetilde{\lambda_{-j}} = \mathcal{O}\left(\frac{1}{\tau^{j/2}}\right), \quad j \geqslant -1.$$

Consequently, the effect of the double asymptotic expansion both in symbols and frequency allows to get some consistent boundary conditions of type:

$$T_{(m+2)} v = \left(\partial_{\mathbf{n}} + \mathrm{i}\mathrm{Op}\left(\sum_{j=-1}^{m} (\widetilde{\lambda_{-j}})_{(m+2)}\right)\right) v = 0, \quad j \geqslant -1, \text{ on } \Sigma,$$

where $(\widetilde{\lambda_{-j}})_{(m+2)}$ designates the Taylor's expansion with respect to the small parameter $\tau^{-1}$ truncated to the term $\tau^{-(m+2)/2}$. The consistency of the conditions results from the equality

$$(\widetilde{\lambda_{-j}})_{(j+2)} = 0.$$

Hence we get the following theorem:

THEOREM 17. – *According to the above controls of the double asymptotic expansion of the total symbol $\widetilde{\lambda}$, the asymptotic consistent artificial boundary condition of order $(m+2)/2$ is given by the following relation*:

$$T_{(m+2)}v = \left(\partial_{\mathbf{n}} + \mathrm{i}\mathrm{Op}\left(\sum_{j=-1}^{m} (\widetilde{\lambda_{-j}})_{(m+2)}\right)\right)v = 0, \quad j \geqslant -1, \text{ on } \Sigma. \tag{41}$$

Taylor's expansion of the principal symbol $\widetilde{\lambda_1}$ implies that the operator defining the above boundary conditions involves some time fractional derivative operators. As a consequence, artificial boundary conditions (41) are *non-local with respect to time*. However, they have the important property of being *local in space* since all the functional $\xi$-dependences are of polynomial type ($\xi$ being the covariable of the curvilinear abscissa $s$). This very fundamental aspect of these new conditions should allow an important gain of the computational time but also of the memory storage required in some numerical experiments.

### 5.2. Computation of the asymptotic artificial boundary conditions

This last part is devoted to the derivation of effective asymptotic artificial boundary conditions of order less than three. Other higher-order conditions can be easily determined by implementing relations (6)–(7) in a computer algebra system. However, because of the complex analytical form of these conditions, we only restrict our study to the first, second and third order conditions. The proposition below gives the asymptotic form of the first six symbols of the asymptotic expansion of symbol $\widetilde{\lambda}$.

PROPOSITION 18. – *The asymptotic expansions of symbols $(\widetilde{\lambda_{-j}})_{-1\leqslant j\leqslant 4}$ in the high-frequency regime and in the $M$-quasi hyperbolic zone $\mathcal{H}$ are given by*:

$$\begin{aligned}
\widetilde{\lambda_1} &= -\mathrm{i}\tau^{1/2} - \frac{1}{2}\mathrm{i}\xi^2\tau^{-1/2} + \frac{\mathrm{i}}{8}\xi^4\tau^{-3/2} + \mathcal{O}(\tau^{-5/2}),\\
\widetilde{\lambda_0} &= \frac{1}{2}\mathrm{i}\kappa - \frac{1}{2}\mathrm{i}\kappa\xi^2\tau^{-1} + \frac{1}{2}\mathrm{i}\kappa\xi^4\tau^{-2} + \mathcal{O}(\tau^{-5/2}),\\
\widetilde{\lambda_{-1}} &= \frac{3}{8}\mathrm{i}\kappa^2\tau^{-1/2} + \frac{1}{16}\mathrm{i}\kappa^2\xi^2\tau^{-3/2} + \mathcal{O}(\tau^{-5/2}),\\
\widetilde{\lambda_{-2}} &= -\frac{1}{8}\mathrm{i}\partial_s^2\kappa\tau^{-1} - \frac{1}{2}\kappa\partial_s\kappa\xi\tau^{-3/2} + \left(\frac{1}{4}\mathrm{i}\kappa^3\xi^2 + \frac{1}{8}\mathrm{i}\partial_s^2\kappa\xi^2\right)\tau^{-2} + \mathcal{O}(\tau^{-5/2}),\\
\widetilde{\lambda_{-3}} &= -\mathrm{i}\left(-\frac{9}{128}\kappa^4 - \frac{3}{8}\kappa\partial_s^2\kappa - \frac{1}{4}(\partial_s\kappa)^2\right)\tau^{-3/2} - \frac{5}{16}\kappa^2\partial_s\kappa\xi\tau^{-2} + \mathcal{O}(\tau^{-5/2}),\\
\widetilde{\lambda_{-4}} &= \left(\frac{1}{2}\mathrm{i}\kappa(\partial_s\kappa)^2 + \frac{11}{32}\mathrm{i}\kappa^2\partial_s^2\kappa + \frac{9}{128}\mathrm{i}\kappa^5\right)\tau^{-2} + \mathcal{O}(\tau^{-5/2}).
\end{aligned}$$

Now, from this proposition and Theorem 17, we can construct the following third-order consistent asymptotic artificial boundary condition.

THEOREM 19. – *The resulting consistent artificial boundary condition of third order in the asymptotic regime is given by*:

$$
\begin{aligned}
&\partial_{\mathbf{n}} u + \mathrm{e}^{-\mathrm{i}\pi/4}\partial_t^{1/2}u - \frac{1}{2}\kappa u - \mathrm{e}^{-\mathrm{i}\pi/4}\left(\frac{1}{2}\Delta_\Gamma + \frac{3}{8}\kappa^2\right)\partial_t^{-1/2}u - \left(\frac{1}{2}\kappa\,\Delta_\Gamma - \frac{1}{8}\Delta_\Gamma\kappa\right)\partial_t^{-1}u \\
&\quad + \mathrm{e}^{\mathrm{i}\pi/4}\left(\left(\frac{1}{8} + \frac{1}{16}\kappa^2\right)\Delta_\Gamma - \frac{1}{2}\kappa\,\partial_s\kappa\,\partial_s - \left(\frac{9}{128}\kappa^4 + \frac{3}{8}\kappa\,\Delta_\Gamma\kappa + \frac{1}{4}\big(\partial_s\kappa\big)^2\right)\right)\partial_t^{-3/2}u \\
&\quad - \mathrm{i}\left(\frac{1}{2}\kappa\,\Delta_\Gamma^2 - \left(\frac{1}{4}\kappa^3 + \frac{1}{8}\Delta_\Gamma\kappa\right)\Delta_\Gamma + \left(\frac{5}{16}\kappa^2\partial_s\kappa\right)\partial_s \right. \\
&\quad \left. + \left(\frac{1}{2}\kappa\big(\partial_s\kappa\big)^2 + \frac{11}{32}\kappa^2\Delta_\Gamma\kappa + \frac{9}{128}\kappa^5\right)\right)\partial_t^{-2}u = 0, \quad \text{on } \Gamma.
\end{aligned}
$$

Hereabove, operator $\partial_t^q$ is the fractional derivative operator of order $q \in \mathbb{Q}^+$ and $\Delta_\Gamma^n = \partial_s^{2n}$ is the Laplace–Beltrami surfacic operator on $\Gamma$ of order $n$, $n \in \mathbb{N}^+$.

We also obtain some artificial conditions of lower integer order.

COROLLARY 20. – *The first-order consistent asymptotic artificial boundary condition is*

$$
\partial_{\mathbf{n}} u + \mathrm{e}^{-\mathrm{i}\pi/4}\partial_t^{1/2}u - \frac{1}{2}\kappa u = 0, \quad \text{on } \Gamma,
$$

*and the second-order one is*

$$
\begin{aligned}
&\partial_{\mathbf{n}} u + \mathrm{e}^{-\mathrm{i}\pi/4}\partial_t^{1/2}u - \frac{1}{2}\kappa u - \mathrm{e}^{-\mathrm{i}\pi/4}\left(\frac{1}{2}\Delta_\Gamma + \frac{3}{8}\kappa^2\right)\partial_t^{-1/2}u \\
&\quad - \left(\frac{1}{2}\kappa\,\Delta_\Gamma - \frac{1}{8}\Delta_\Gamma\kappa\right)\partial_t^{-1}u = 0, \quad \text{on } \Gamma.
\end{aligned}
$$

*Remark* 5. – We do not adress here the problem of well-posedness of the resulting asymptotic boundary value problem with one of the previous conditions. It is well known that the problem is a hard task as exemplified, e.g., in [11,12,24].

Let us note that other approximations may lead to other possible artificial conditions. For example, we can mention the approach of paraxial approximations techniques [9,10,23,25] which yields other families of artificial conditions (which should be "more local" than the above ones). However, this issue is beyond the scope of the paper. This point as well as the numerical approximation and efficiency of the above conditions in some physical situations will be analyzed and developed in a forthcoming work.

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